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LOGINID:SSPTANXR1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	DEC 01	ChemPort single article sales feature unavailable
NEWS 3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 4	APR 07	STN is raising the limits on saved answers
NEWS 5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS 6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS 7	APR 28	CAS patent authority coverage expanded
NEWS 8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS 10	MAY 08	STN Express, Version 8.4, now available
NEWS 11	MAY 11	STN on the Web enhanced
NEWS 12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS 13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS 14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS 15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS 16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS 17	JUN 26	NUTRACEUT and PHARMAML no longer updated
NEWS 18	JUN 29	IMSCOPROFILE now reloaded monthly
NEWS 19	JUN 29	EPFULL adds Simultaneous Left and Right Truncation (SLART) to AB, MCLM, and TI fields
NEWS 20	JUL 09	PATDPAFULL adds Simultaneous Left and Right Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS 21	JUL 14	USGENE enhances coverage of patent sequence location (PSL) data
NEWS 22	JUL 14	CA/CAplus to be enhanced with new citing references features
NEWS 23	JUL 16	GBFULL adds patent backfile data to 1855

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:48:38 ON 20 JUL 2009

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 18:48:46 ON 20 JUL 2009
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5
DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804.str

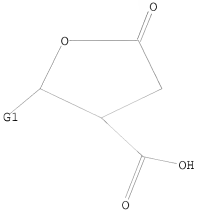
chain nodes :
6 7 8 9 12
ring nodes :
1 2 3 4 5
chain bonds :
1-7 2-12 4-6 7-8 7-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-12 4-6
exact bonds :
1-2 1-5 1-7 2-3 3-4 4-5
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

G1:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
12:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 18:49:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1817 TO ITERATE

100.0% PROCESSED 1817 ITERATIONS 604 ANSWERS
SEARCH TIME: 00.00.01

L2 604 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'CAPLUS' ENTERED AT 18:49:11 ON 20 JUL 2009
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FILE COVERS 1907 - 20 Jul 2009 VOL 151 ISS 4

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FILE LAST UPDATED: 19 Jul 2009  (20090719/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Jun 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family
of databases will soon be updated to include new citing references
information.  This enhancement may impact record import into
database management software.  For additional information, refer
to NEWS 22.

=> s l2 full
L3          757 L2

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       1.00     187.10

FILE 'REGISTRY' ENTERED AT 18:50:09 ON 20 JUL 2009
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STRUCTURE FILE UPDATES:   19 JUL 2009  HIGHEST RN 1165441-73-5
DICTIONARY FILE UPDATES:  19 JUL 2009  HIGHEST RN 1165441-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804a.str
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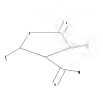


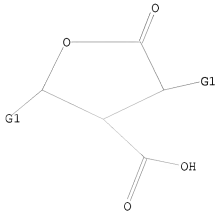
chain nodes :
6 7 8 9 12 13
ring nodes :
1 2 3 4 5
chain bonds :
1-7 2-12 4-6 5-13 7-8 7-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-12 4-6 5-13
exact bonds :
1-2 1-5 1-7 2-3 3-4 4-5
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

G1:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
12:CLASS 13:CLASS

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
FULL SEARCH INITIATED 18:50:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1817 TO ITERATE

100.0% PROCESSED 1817 ITERATIONS 183 ANSWERS
SEARCH TIME: 00.00.01

L5 183 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 372.98

FILE 'CAPLUS' ENTERED AT 18:50:44 ON 20 JUL 2009
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FILE COVERS 1907 - 20 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 19 Jul 2009 (20090719/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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of databases will soon be updated to include new citing references
information. This enhancement may impact record import into
database management software. For additional information, refer
to NEWS 22.

=> s l5 full
L6   142 L5

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   1.50   374.48

FILE 'REGISTRY' ENTERED AT 18:52:27 ON 20 JUL 2009
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STRUCTURE FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5
DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804b.str

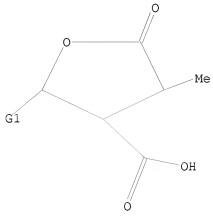
chain nodes :
6 7 8 9 12 13
ring nodes :
1 2 3 4 5
chain bonds :
1-7 2-12 4-6 5-13 7-8 7-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-12 4-6
exact bonds :
1-2 1-5 1-7 2-3 3-4 4-5 5-13
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

G1:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
12:CLASS 13:CLASS

L7 STRUCTURE UPLOADED

=> d 17
L7 HAS NO ANSWERS
L7 STR



G1 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l7 full
FULL SEARCH INITIATED 18:52:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 798 TO ITERATE

100.0% PROCESSED 798 ITERATIONS 100 ANSWERS
SEARCH TIME: 00.00.01

L8 100 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 560.36

FILE 'CAPLUS' ENTERED AT 18:52:57 ON 20 JUL 2009
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FILE COVERS 1907 - 20 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 19 Jul 2009 (20090719/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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information. This enhancement may impact record import into
database management software. For additional information, refer
to NEWS 22.

=> s l8 full
L9   97 L8

=> s l6 not l9
L10   45 L6 NOT L9

=> d ibib abs hitstr tot

L10 ANSWER 1 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:257303 CAPLUS

DOCUMENT NUMBER: 150:438336

TITLE: C75 is converted to C75-CoA in the hypothalamus, where it inhibits carnitine palmitoyltransferase 1 and decreases food intake and body weight

AUTHOR(S): Mera, Paula; Bentebibel, Assia; Lopez-Vinas, Eduardo; Cordente, Antonio G.; Gurunathan, Chandrashekaran; Sebastian, David; Vazquez, Irene; Herrero, Laura; Ariza, Xavier; Gomez-Puertas, Paulino; Asins, Guillermina; Serra, Dolors; Garcia, Jordi; Hegardt, Fausto G.

CORPORATE SOURCE: Department of Biochemistry and Molecular Biology and IBUB (Institute of Biomedicine), University of Barcelona, Spain

SOURCE: Biochemical Pharmacology (2009), 77(6), 1084-1095
CODEN: BCPCA6; ISSN: 0006-2952

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Central nervous system administration of C75 produces hypophagia and weight loss in rodents identifying C75 as a potential drug against obesity and type 2 diabetes. However, the mechanism underlying this effect is unknown. C75-CoA is generated chemical, in vitro and in vivo from C75 and that it is a potent inhibitor of carnitine palmitoyltransferase 1 (CPT1), the rate-limiting step of fatty-acid oxidation Three-D docking and kinetic anal. support the inhibitory effect of C75-CoA on CPT1. Central nervous system administration of C75 in rats led to C75-CoA production, inhibition of CPT1 and lower body weight and food intake. The authors' results suggest that inhibition of CPT1, and thus increased availability of fatty acids in the hypothalamus, contribute to the pharmacol. mechanism of C75 to decrease food intake.

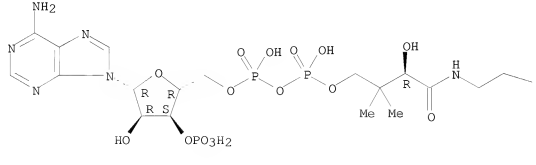
IT 1145878-63-2P
RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)
(C75 is converted to C75-CoA in hypothalamus, where it inhibits carnitine palmitoyltransferase 1 and decreases food intake and body weight)

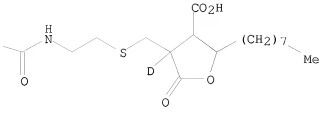
RN 1145878-63-2 CAPLUS

CN Coenzyme A, S-[(4-carboxytetrahydro-5-octyl-2-oxo-3-furanyl-3-d)methyl]- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

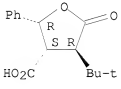
L10 ANSWER 2 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:286862 CAPLUS
DOCUMENT NUMBER: 143:7261
TITLE: Dialkylzinc mediated radical additions to chiral N-enoyloxazolidinones in the presence of benzaldehyde. Mechanistic investigation, structural characterization of the resulting γ-lactones
AUTHOR(S): Bazin, Samantha; Feray, Laurence; Vanthuyne, Nicolas; Bertrand, Michele P.
CORPORATE SOURCE: Laboratoire de Chimie Moleculaire Organique--UMR 6517, Faculte des Sciences St. Jerome, Universite d'Aix-Marseille III, Marseille, 13397, Fr.
SOURCE: Tetrahedron (2005), 61(17), 4261-4274
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7261

AB Diethylzinc was used in the presence of oxygen to mediate radical addns. to chiral N-enoyloxazolidinones derived from fumaric acid. The synthesis of sterically crowded trisubstituted γ-lactones was achieved through a multicomponent reaction involving t-Bu iodide and benzaldehyde in addition to the above mentioned reagents. The domino process includes successively: iodine atom transfer, radical addition, homolytic substitution at zinc, aldol condensation, and lactonization. The diastereoselectivity of the reaction and the structural features of the resulting lactones were investigated. A tentative rationalization is discussed. Comparative expts. carried out with diisopropylzinc were performed.

IT 852487-24-2P 852487-34-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction mechanism on dialkylzinc mediated radical addns. to chiral N-enoyloxazolidinones in presence of benzaldehyde and structural characterization of resulting γ-lactones)

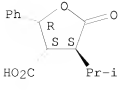
RN 852487-24-2 CAPLUS
CN 3-Furancarboxylic acid, 4-(1,1-dimethylethyl)tetrahydro-5-oxo-2-phenyl-, (2R,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



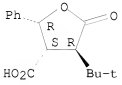
RN 852487-34-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-methylethyl)-5-oxo-2-phenyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.



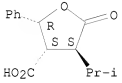
IT 852487-38-8P 852487-44-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction mechanism on dialkylzinc mediated radical addns. to chiral N-enoyloxazolidinones in presence of benzaldehyde and structural characterization of resulting γ-lactones)
RN 852487-38-8 CAPLUS
CN 3-Furancarboxylic acid, 4-(1,1-dimethylethyl)tetrahydro-5-oxo-2-phenyl-, (2R,3S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



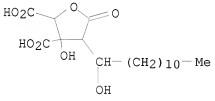
RN 852487-44-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-methylethyl)-5-oxo-2-phenyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

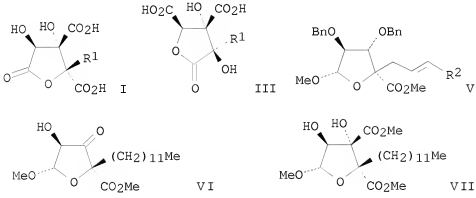


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:831435 CAPLUS
DOCUMENT NUMBER: 139:396091
TITLE: New avenues in nitrenium ion and carbene chemistry: total synthesis of TAN 1251A, cinatrin B, C1, and C
AUTHOR(S): Basak, Arindrajit
CORPORATE SOURCE: Univ. of Illinois, Chicago, IL, USA
SOURCE: (2002) 263 pp. Avail.: UMI, Order No. DA3074129
From: Diss. Abstr. Int., B 2003, 63(12), 5843
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 136266-36-9P, Cinatrin C2
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. total synthesis of TAN 1251A, cinatrin N, C1, and C via the use of a nitrenium ion spirocyclization and intramol. CH insertion reactions)
RN 136266-36-9 CAPLUS
CN Pentaric acid, 3-C-carboxy-2-deoxy-2-(1-hydroxydodecyl)-, 1,4-lactone (9CI) (CA INDEX NAME)



L10 ANSWER 4 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:800317 CAPLUS
DOCUMENT NUMBER: 140:76919
TITLE: Enantiospecific synthesis of the phospholipase A2 inhibitors (-)-cinatrin C1 and (+)-cinatrin C3
AUTHOR(S): Cuzzupe, Anthony N.; Di Florio, Romina; White, Jonathan M.; Rizzacasa, Mark A.
CORPORATE SOURCE: School of Chemistry, The University of Melbourne, Victoria, 3010, Australia
SOURCE: Organic & Biomolecular Chemistry (2003), 1(20), 3572-3577
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76919
GI



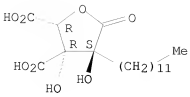
AB The enantiospecific synthesis of (-)-cinatrin C1 [I; R1 = (CH2)11Me (II)] and (+)-cinatrin C3 [III; R1 = (CH2)11Me (IV)] from the D-arabinose derivative V [R2 = (CH2)8Me] is described. The stereochem. at C2 was introduced via a chelation-controlled addition of a carbanion to α-hydroxy ketone (VI). The best selectivity was achieved by use of the Grignard reagent derived from trimethylsilylacetylene. Transformation of the terminal alkyne into Me ester VII followed by acetal hydrolysis and selective lactol oxidation gave cinatrin C1 di-Me ester. Base hydrolysis and acid induced relactonization then gave a 1 : 1 mixture of II and IV.

IT 136266-37-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cinatrin C1 and cinatrin C3 utilizing chelation-controlled addition of a carbanion to α-hydroxyketone as a key step)

RN 136266-37-0 CAPLUS

CN D-Xylaric acid, 3-C-carboxy-2-C-dodecyl-, 1,4-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

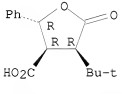
L10 ANSWER 5 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:808596 CAPLUS
DOCUMENT NUMBER: 138:187268
TITLE: Tandem radical addition-aldol condensations: evidence for the formation of zinc enolates in diethyl zinc mediated radical additions to N-enoyloxazolidinones
AUTHOR(S): Bazin, S.; Feray, L.; Siri, D.; Naubron, J.-V.; Bertrand, Michele P.
CORPORATE SOURCE: Laboratoire de Chimie Moleculaire Organique, UMR 6517, Boite 562, Faculte des Sciences St Jerome, Universite d'Aix-Marseille III, Av. Escadrille Normandie-Niemen, 13397 Marseille, Fr.
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (21), 2506-2507
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187268

AB Diethylzinc mediated addition of alkyl radicals to chiral N-enoyloxazolidinones is immediately followed by homolytic substitution at zinc leading to a zinc enolate; the trapping of the latter in a subsequent aldol condensation serves as a useful mechanistic probe; overall this reaction sequence constitutes a novel example of a one pot, three-component, radical-polar crossover reaction.

IT 499130-73-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(aldol condensations of zinc enolates formation in di-Et zinc mediated radical addns. to enoyloxazolidinones)

RN 499130-73-3 CAPLUS
CN 3-Furancarboxylic acid, 4-(1,1-dimethylethyl)tetrahydro-5-oxo-2-phenyl-, (2R,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:732352 CAPLUS
DOCUMENT NUMBER: 130:81762
TITLE: A symmetry-based approach to zaragozic acid: synthesis and end-differentiation of an advanced intermediate
AUTHOR(S): Freeman-Cook, Kevin D.; Halcomb, Randall L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Univ. of Colorado, Boulder, CO, 80309-0215, USA
SOURCE: Tetrahedron Letters (1998), 39(47), 8567-8570
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:81762

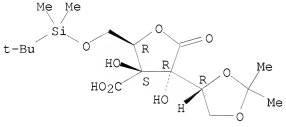
AB Reported is a novel, symmetry-based strategy for the synthesis of the zaragozic acids. Two enantioselective dihydroxylations are used to set the absolute stereochem. of a C-2 sym. intermediate. A sequence of a furan photo-oxidation followed by a diastereoselective dihydroxylation breaks the symmetry and sets two quaternary stereo-centers. Finally, a group selective lactonization is used to protect one of two secondary hydroxyls. This accomplishes the critical end-differentiation of this intermediate. An approach to protecting group removal and oxidation is also presented.

IT 218767-23-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and end-differentiation of an advanced intermediate in the synthesis of zaragozic acid)

RN 218767-23-8 CAPLUS

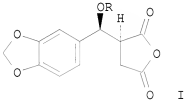
CN 3-Furancarboxylic acid, 4-[(4R)-2,2-dimethyl-1,3-dioxolan-4-yl]-2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]tetrahydro-3,4-dihydroxy-5-oxo-, (2R,3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:14135 CAPLUS
DOCUMENT NUMBER: 128:127855
ORIGINAL REFERENCE NO.: 128:25115a,25118a
TITLE: New synthesis of 2,6-diaryl-4-oxo-3,7-dioxabicyclo[3.3.0]octanes. Synthesis of (±)-styraxin
AUTHOR(S): Yoshida, Shinichi; Ogiku, Tsuyoshi; Ohmizu, Hiroshi; Iwasaki, Tameo
CORPORATE SOURCE: Lead Optimization Research Laboratory, Tanabe Seiyaku Co. Ltd., Kashima, 532, Japan
SOURCE: Synthesis (1997), (12), 1475-1480
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:127855
GI



I

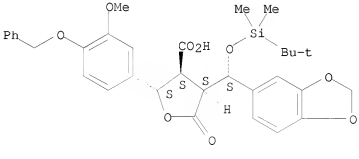
AB An efficient method for the stereocontrolled synthesis of a 4-oxofurofuran lignan, (±)-styraxin was developed based on the stereocontrolled aldol reaction of the succinic anhydride I (R = SiMe2CMe3) with benzylvanillin.

IT 201747-96-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of styraxin)

RN 201747-96-8 CAPLUS

CN 3-Furancarboxylic acid, 4-[(R)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]tetrahydro-2-[3-methoxy-4-(phenylmethoxy)phenyl]-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



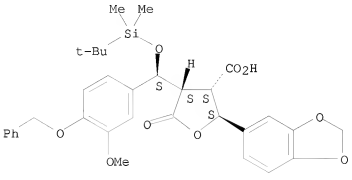
IT 201747-93-5P 201747-94-6P 201747-95-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of styraxin)

RN 201747-93-5 CAPLUS

CN 3-Furancarboxylic acid, 2-(1,3-benzodioxol-5-yl)-4-[(R)-[[(1,1-dimethylethyl)dimethylsilyl]oxy][3-methoxy-4-

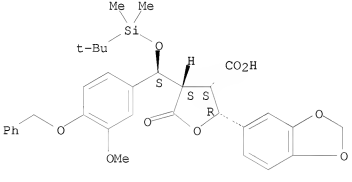
(phenylmethoxy)phenyl]methyl]tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



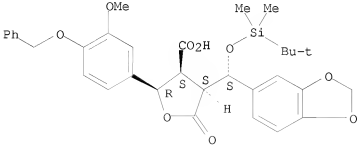
RN 201747-94-6 CAPLUS
CN 3-Furancarboxylic acid, 2-(1,3-benzodioxol-5-yl)-4-[(S)-[[(1,1-dimethylethyl)dimethylsilyl]oxy][3-methoxy-4-(phenylmethoxy)phenyl]methyl]tetrahydro-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 201747-95-7 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]tetrahydro-2-[3-methoxy-4-(phenylmethoxy)phenyl]-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



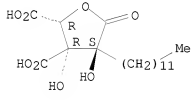
L10 ANSWER 8 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:439248 CAPLUS
DOCUMENT NUMBER: 127:176283
ORIGINAL REFERENCE NO.: 127:34151a,34154a
TITLE: Aldol reactions of ketal-protected tartrate ester enolates. Asymmetric syntheses and absolute stereochemical assignments of phospholipase A2 inhibitors cinatrin C1 and C3
AUTHOR(S): Evans, David A.; Trotter, B. Wesley; Barrow, James C.
CORPORATE SOURCE: Department of Chemistry & Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Tetrahedron (1997), 53(26), 8779-8794
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An efficient approach to the syntheses of cinatrins C1 and C3 has been developed and used to establish the absolute configurations of these natural products. The construction of each mol. has been achieved in a five-step reaction sequence (overall yield 43% for cinatrin C1, 33% for cinatrin C3) from the di-tert-Bu ester of (R,R)-tartaric acid. The two contiguous, quaternary chiral centers in the cinatrin skeleton are constructed via a diastereoselective, titanium-mediated aldol coupling of a tartrate-derived silylketene acetal and an achiral α-ketoester. This bond construction proceeds with excellent diastereoselectivity for a variety of aldehyde and α-ketoester substrates.

IT 136266-37-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(asym. syntheses by aldol reactions of ketal-protected tartrate ester enolates and absolute stereochem. assignments of phospholipase A2 inhibitors cinatrin C1 and C3)

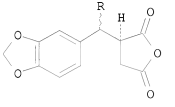
RN 136266-37-0 CAPLUS
CN D-Xylaric acid, 3-C-carboxy-2-C-dodecyl-, 1,4-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.

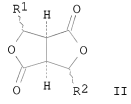


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:210829 CAPLUS
DOCUMENT NUMBER: 126:185933
ORIGINAL REFERENCE NO.: 126:35901a,35904a
TITLE: First Stereocontrolled Syntheses of Unsymmetrically Substituted Bislactone Lignans: Stereocontrolled Syntheses of Four Possible Isomers of Methyl 4,8-Dioxoxanthoxylol
AUTHOR(S): Yoshida, Shin-ichi; Ogiku, Tsuyoshi; Ohmizu, Hiroshi; Iwasaki, Tameo
CORPORATE SOURCE: Lead Optimization Research Laboratory, Tanabe Seiyaku Co. Ltd., Osaka, 532, Japan
SOURCE: Journal of Organic Chemistry (1997), 62(5), 1310-1316
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:185933
GI



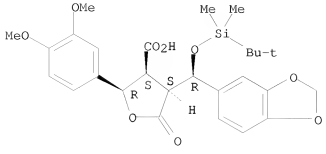
I



II

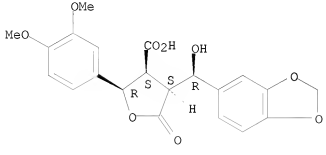
AB An efficient method for stereocontrolled syntheses of the unsym. substituted bislactone subgroup of the furofuran lignan was developed based on a stereoselective aldol reaction of the acid anhydrides I (R = α-, β-OSiMe2CMe3) with an aromatic aldehyde, i.e. veratraldehyde, for the preparation of Me 4,8-dioxoxanthoxylol II (R1 = β-3,4-methylenedioxyphenyl, R2 = α-3,4-dimethoxyphenyl), 4,8-dioxofargesin II (R1 = β-3,4-dimethoxyphenyl, R2 = α-3,4-methylenedioxyphenyl), Me 4,8-dioxopiperitol II (R1 = α-3,4-methylenedioxyphenyl, R2 = α-3,4-dimethoxyphenyl) and their isomer II (R1 = β-3,4-methylenedioxyphenyl, R2 = β-3,4-dimethoxyphenyl) as the representative examples of the axial-equatorial, diequatorial, and diaxial types of this series.
IT 171296-45-0P 171296-47-2P 187604-21-3P
187604-24-6P 187604-26-8P 187604-28-0P
187604-30-4P 187604-32-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective syntheses of diastereoisomers of Me 4,8-dioxoxanthoxylol)
RN 171296-45-0 CAPLUS
CN 3-Furancarboxylic acid, 4-[1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, [2α,3α,4α(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



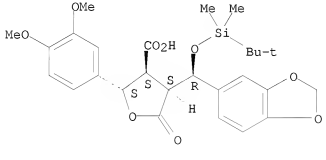
RN 171296-47-2 CAPLUS
CN 3-Furancarboxylic acid, 4-(1,3-benzodioxol-5-ylhydroxymethyl)-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, [2α,3α,4α(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



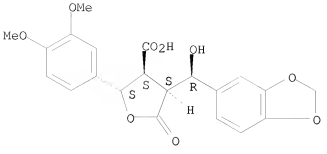
RN 187604-21-3 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



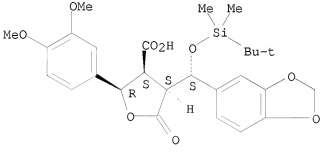
RN 187604-24-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-ylhydroxymethyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



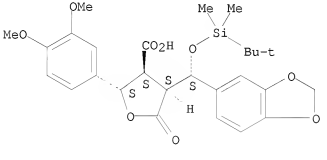
RN 187604-26-8 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



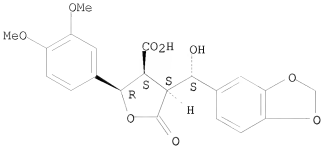
RN 187604-28-0 CAPLUS
CN 3-Furancarboxylic acid, 4-[(R)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



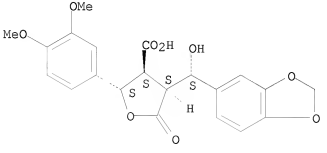
RN 187604-30-4 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-ylhydroxymethyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



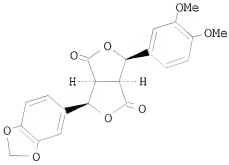
RN 187604-32-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[(R)-1,3-benzodioxol-5-ylhydroxymethyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:913178 CAPLUS
DOCUMENT NUMBER: 124:29504
ORIGINAL REFERENCE NO.: 124:5659a,5662a
TITLE: The first synthesis of diaxial bislactone furofuran lignan
AUTHOR(S): Yoshida, Shin-ichi; Ohmizu, Hiroshi; Iwasaki, Tameo
CORPORATE SOURCE: Lead Optimization Res. Lab., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan
SOURCE: Tetrahedron Letters (1995), 36(45), 8225-6
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:29504
GI



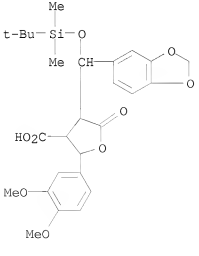
I

AB The diaxial bislactone furofuran lignan I was synthesized via a stereocontrolled aldol reaction of the acid anhydride and veratraldehyde.

IT 171296-46-1P
RL: BYP (Byproduct); PREP (Preparation)
(synthesis of diaxial bislactone furofuran lignan)

RN 171296-46-1 CAPLUS

CN 3-Furancarboxylic acid, 4-[1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo- (CA INDEX NAME)

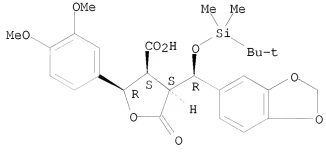


IT 171296-45-0P 171296-47-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of diaxial bislactone furofuran lignan)

RN 171296-45-0 CAPLUS

CN 3-Furancarboxylic acid, 4-[1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, [2α,3α,4α(R*)]- (9CI) (CA INDEX NAME)

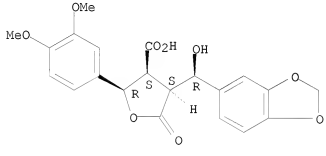
Relative stereochemistry.



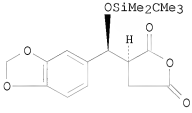
RN 171296-47-2 CAPLUS

CN 3-Furancarboxylic acid, 4-(1,3-benzodioxol-5-ylhydroxymethyl)-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, [2α,3α,4α(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L10 ANSWER 11 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:419458 CAPLUS
DOCUMENT NUMBER: 122:290560
ORIGINAL REFERENCE NO.: 122:52971a,52974a
TITLE: The first stereocontrolled synthesis of diequatorial bislactone furofuran lignans having two different aryl groups: a synthesis of methyl 4,8-dioxopiperitol
AUTHOR(S): Yoshida, Shinichi; Ogiku, Tsuyoshi; Ohmizu, Hiroshi; Iwasaki, Tameo
CORPORATE SOURCE: Res. Lab. Appl. Biochem., Tanabe Seiyaku Co., Ltd., Kashima, 532, Japan
SOURCE: Tetrahedron Letters (1995), 36(9), 1459-60
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:290560
GI



I

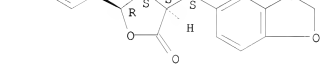
AB Me 4,8-dioxopiperitol, a representative example of the diequatorial bislactone furofuran lignans having two different aryl groups, was synthesized based on the stereocontrolled aldol reaction of the acid anhydride I and veratral.

IT 187604-26-8P
RL: BYP (Byproduct); PREP (Preparation)
(stereoselective synthesis of Me 4,8-dioxopiperitol)

RN 187604-26-8 CAPLUS

CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

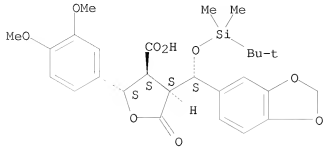


IT 187604-28-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of Me 4,8-dioxopiperitol)

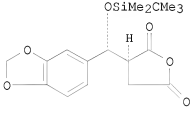
RN 187604-28-0 CAPLUS

CN 3-Furancarboxylic acid, 4-[(R)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



L10 ANSWER 12 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:419457 CAPLUS
DOCUMENT NUMBER: 122:290559
ORIGINAL REFERENCE NO.: 122:52971a,52974a
TITLE: The first stereocontrolled synthesis of axial-equatorial bislactone furofuran lignans having two different aryl groups: a synthesis of methyl 4,8-dioxoxanthoxylol
AUTHOR(S): Yoshida, Shinichi; Ogiku, Tsuyoshi; Ohmizu, Hiroshi; Iwasaki, Tameo
CORPORATE SOURCE: Res. Lab. Appl. Biochem., Tanabe Seiyaku Co., Ltd., Osaka, 532, Japan
SOURCE: Tetrahedron Letters (1995), 36(9), 1455-8
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:290559
GI



I

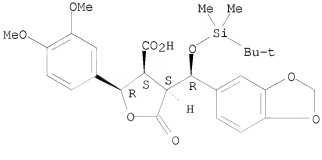
AB Me 4,8-dioxoxanthoxylol, a prepresentative example of the axial-equatorial bislactone furofuran lignans having two different aryl groups, was synthesized based on the stereocontrolled aldol reaction of the acid anhydride I and veratral.

IT 171296-45-0P
RL: BYP (Byproduct); PREP (Preparation)
(stereoselective synthesis of Me dioxoxanthoxylolol)

RN 171296-45-0 CAPLUS

CN 3-Furancarboxylic acid, 4-[1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, [2α,3α,4α(R*)]- (9CI) (CA INDEX NAME)

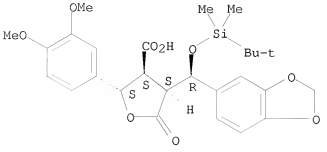
Relative stereochemistry.



IT 187604-21-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of Me dioxoxanthoxylolol)

RN 187604-21-3 CAPLUS
CN 3-Furancarboxylic acid, 4-[(S)-1,3-benzodioxol-5-yl[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-(3,4-dimethoxyphenyl)tetrahydro-5-oxo-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

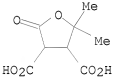


L10 ANSWER 13 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:401083 CAPLUS
DOCUMENT NUMBER: 123:169252
ORIGINAL REFERENCE NO.: 123:30203a,30206a
TITLE: Synthesis of pyrethrin precursors and methylene lactones by decarboxylation of 1,1,2-cyclopropanetricarboxylic acids
AUTHOR(S): Benayache, S.; Benayache, F.; Jullien, R. F.; Wanat, M.
CORPORATE SOURCE: Inst. Chimie, Univ. de Constantine, Constantine, 25000, Algeria
SOURCE: Journal de la Societe Algerienne de Chimie (1992), 2(2), 99-110
CODEN: JSACEX; ISSN: 1111-4797
PUBLISHER: Societe Algerienne de Chimie
DOCUMENT TYPE: Journal
LANGUAGE: French

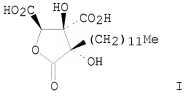
AB Cyclopropanetricarboxylic acids underwent decarboxylation in aprotic solvents. Cyclopropane ring opening occurs under acidic conditions. Thus, 3,3-dimethyl-1,1,2-cyclopropanetricarboxylic acid was treated with NaH in HMPT or 10% H2SO4 to afford cis- and trans-3,3-dimethyl-1,2-cyclopropanedicarboxylic acid or γ,γ-dimethyl-α,β-dicarboxy-γ-butyrolactone, resp.

IT 167283-42-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of pyrethrin precursors and methylene lactones by decarboxylation of cyclopropanetricarboxylic acids)

RN 167283-42-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2,2-dimethyl-5-oxo- (CA INDEX NAME)



L10 ANSWER 14 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:424254 CAPLUS
DOCUMENT NUMBER: 119:24254
ORIGINAL REFERENCE NO.: 119:4421a,4424a
TITLE: Cinatrins, a novel family of phospholipase A2 inhibitors. I. Taxonomy and fermentation of the producing culture; isolation and structures of cinatrins
AUTHOR(S): Itazaki, Hiroshi; Nagashima, Kazuo; Kawamura, Yoshimi; Matsumoto, Koichi; Nakai, Hiroshi; Terui, Yoshihiro
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Antibiotics (1992), 45(1), 38-49
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

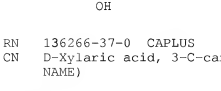


I

AB Cinatrins A, B, C1, C2, and C3 (I), a family of phospholipase A2 inhibitors, were isolated from the fermentation broth of Circinotrichum falcatisporum RF-641. They are novel spiro-γ-dilactones and γ-lactones derived from 1,2,3,5-tetra or 1,2,3(or 1,2,4)-trihydroxypentadecane-1,2,3-tricarboxylic acids. Structures were elucidated by MS and NMR studies and chemical transformations. The structure of I was confirmed by x-ray crystallog. anal., and its absolute configuration was determined by comparison of the CD spectra with related compds.

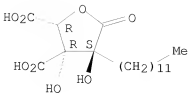
IT 136266-36-9, Cinatrin C2 136266-37-0, Cinatrin C3
RL: BIOL (Biological study)
(from Circinotrichum falcatisporum)

RN 136266-36-9 CAPLUS
CN Pentaric acid, 3-C-carboxy-2-deoxy-2-(1-hydroxydodecyl)-, 1,4-lactone (9CI) (CA INDEX NAME)



RN 136266-37-0 CAPLUS
CN D-Xylaric acid, 3-C-carboxy-2-C-dodecyl-, 1,4-lactone (9CI) (CA INDEX NAME)

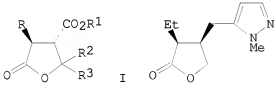
Absolute stereochemistry.


HO2C
O
O
R
R
S
Me
HO2C
(CH2)11
HO
HO

L10 ANSWER 15 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:192080 CAPLUS
DOCUMENT NUMBER: 118:192080
ORIGINAL REFERENCE NO.: 118:33013a,33016a
TITLE: Synthesis of optically active lactones from l-aspartic acid and intermediates thereof
INVENTOR(S): Rapoport, Henry; Dener, Jeffrey M.; Zhang, Lin Hua Zhang
PATENT ASSIGNEE(S): University of California, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9221675	A1	19921210	WO 1992-US3822	19920507
W: AU, BB, BG, BR, CA, FI, HU, JP, KP, KR, LK, MG, MW, NO, PL, RO, RU, SD				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
US 5322942	A	19940621	US 1991-709373	19910603
CA 2110572	A1	19921210	CA 1992-2110572	19920507
AU 9220266	A	19930108	AU 1992-20266	19920507
AU 664559	B2	19951123		
JP 06508136	T	19940914	JP 1992-500417	19920507
EP 643710	A1	19950322	EP 1992-913640	19920507
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
NO 9304376	A	19931202	NO 1993-4376	19931202
PRIORITY APPLN. INFO.:			US 1991-709373 A	19910603
			WO 1992-US3822 A	19920507

OTHER SOURCE(S): MARPAT 118:192080
GI



I II III

AB Optically active lactones I (R, R1 = C1-6 alkyl, C6-10 cycloalkyl, C6-10 aryl, C7-19 arylalkyl; R2 = H, C1-6 alkyl; R3 = homo- or heteroarom. ring with 5 or 6 ring atoms being substituted by C1-6, alkoxy, halo, cyano, nitro) were prepared from L-aspartic acid and can be readily converted to (+)-pilocarpine (II) and analogs by hydrolysis, reduction and hydrogenation. Thus, (2S,3S)-dimethyl 2-bromo-3-ethylsuccinate prepared in 9 steps from L-aspartic acid underwent aldol reaction with 1-methyl-9-imidazolecarboxaldehyde in presence of a zinc-silver couple, CuBr and Me2AlCl to give 94% imidazolylfuranone III, and the corresponding cis isomer (91:9). III underwent hydrogenation in presence of Pd in MeOH followed LiBH4 induced lactonization to give II.

IT 146849-32-3P 146849-35-6P 146849-36-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

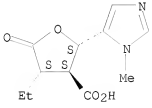
RN 146849-32-3 CAPLUS

CN 3-Furancarboxylic acid, 4-ethyltetrahydro-2-(1-methyl-1H-imidazol-5-yl)-5-oxo-, [2S-(2α,3β,4α)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 146849-31-2
CMF C11 H14 N2 O4

Absolute stereochemistry.



CM 2

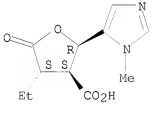
CRN 76-05-1
CMF C2 H F3 O2

RN 146849-35-6 CAPLUS
CN 3-Furancarboxylic acid, 4-ethyltetrahydro-2-(1-methyl-1H-imidazol-5-yl)-5-oxo-, [2R-(2α,3α,4β)]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 146849-34-5
CMF C11 H14 N2 O4

Absolute stereochemistry.



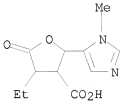
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 146849-36-7 CAPLUS
CN 3-Furancarboxylic acid, 4-ethyltetrahydro-2-(1-methyl-1H-imidazol-5-yl)-5-oxo-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

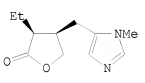
CRN 146500-03-0
CMF C11 H14 N2 O4



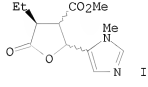
CM 2

CRN 76-05-1
CMF C2 H F3 O2

L10 ANSWER 16 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:169391 CAPLUS
DOCUMENT NUMBER: 118:169391
ORIGINAL REFERENCE NO.: 118:29061a,29064a
TITLE: An effective chirospecific synthesis of (+)-pilocarpine from L-aspartic acid
AUTHOR(S): Dener, Jeffrey M.; Zhang, Lin Hua; Rapoport, Henry
CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Journal of Organic Chemistry (1993), 58(5), 1159-66
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 118:169391
GI

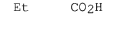


I

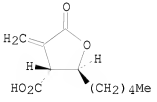


II

AB A short and efficient synthesis of (+)-pilocarpine (I) has been accomplished in 10 steps and 51% overall yield from L-aspartic acid. The synthesis features a diastereoselective alkylation of a protected aspartic acid diester derivative and a selective hydrolysis of the α-Me ester to give the corresponding amino acid. Subsequent replacement of the amino group with bromo, esterification, and a modified Reformatskii reaction with 1-methylimidazole-5-carboxaldehyde afforded imidazole-substituted lactone II. Details concerning this novel lactones synthesis are also described. Finally, hydrogenolysis of the lactone carbon-oxygen bond and selective reduction of the resulting monoester afforded pure (+)-pilocarpine.
IT 146500-03-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, conversion to acid chloride, and reduction of)
RN 146500-03-0 CAPLUS
CN 3-Furancarboxylic acid, 4-ethyltetrahydro-2-(1-methyl-1H-imidazol-5-yl)-5-oxo- (CA INDEX NAME)

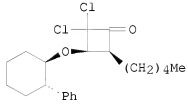


L10 ANSWER 17 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:490013 CAPLUS
DOCUMENT NUMBER: 117:90013
ORIGINAL REFERENCE NO.: 117:15705a,15708a
TITLE: Novel, enantioselective lactone construction. First synthesis of methylenolactocin, antitumor antibiotic from Penicillium sp
AUTHOR(S): De Azevedo, Mariangela B. M.; Murta, Maria M.; Greene, Andrew E.
CORPORATE SOURCE: Univ. Joseph Fourier Grenoble, Grenoble, 38041, Fr.
SOURCE: Journal of Organic Chemistry (1992), 57(17), 4567-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:90013
GI



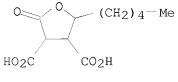
I

II



III

AB The first synthesis of (-)-methylenolactocin (I), an antitumor antibiotic isolated from the culture filtrate of Penicillium sp., was achieved from the cyclohexanol II via Baeyer-Villiger oxidation of the cyclobutanone III. The work illustrates a novel and potentially general approach to enantiopure γ-butyrolactones based on π-face differentiation in chiral olefin-ketene [2+2]-cycloaddn. The synthesis serves to confirm the structure and establish the absolute stereochem. of natural I and, also, to demonstrate a significantly improved procedure for the conversion of γ-butyrolactones to the important α-methylene derivs.
IT 142188-52-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylative methylenation of)
RN 142188-52-1 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-pentyl- (CA INDEX NAME)

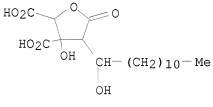


L10 ANSWER 18 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:230606 CAPLUS
DOCUMENT NUMBER: 116:230606
ORIGINAL REFERENCE NO.: 116:38931a,38934a
TITLE: Cinatrins, a novel family of phospholipase A2 inhibitors. II. Biological activities
AUTHOR(S): Tanaka, Kazushige; Itazaki, Hiroshi; Yoshida, Tadashi
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Antibiotics (1992), 45(1), 50-5
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cinatrins A, B, and C3 inhibited phospholipase A2 purified from rat blood platelets in a dose-dependent manner. Cinatrin C3, the most potent component (IC50 = 70 μM), was noncompetitive with a Ki of 36 μM. Cinatrins B and C3 also inhibited both porcine pancreas and Naja naja venom phospholipases A2. Inhibition of rat platelet phospholipase A2 by cinatrin C3 was independent of Ca2+ and the substrate concentration Comparison with duramycin, another phospholipase A2 inhibitor, displayed inhibition dependent on substrate concentration when phosphatidylethanolamine was the substrate. The results indicated that the inhibition of phospholipase A2 by cinatrin C3 may result from direct interaction with the enzyme.

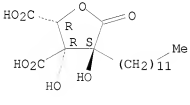
IT 136266-36-9, Cinatrin C2 136266-37-0, Cinatrin C3
RL: BIOL (Biological study)
(phospholipases A2 of blood platelets and other sources inhibition by, kinetics of, structure in relation to)

RN 136266-36-9 CAPLUS
CN Pentaric acid, 3-C-carboxy-2-deoxy-2-(1-hydroxydodecyl)-, 1,4-lactone (9CI) (CA INDEX NAME)



RN 136266-37-0 CAPLUS
CN D-Xylaric acid, 3-C-carboxy-2-C-dodecyl-, 1,4-lactone (9CI) (CA INDEX NAME)

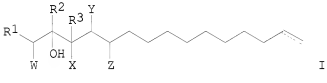
Absolute stereochemistry.



L10 ANSWER 19 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:557127 CAPLUS
DOCUMENT NUMBER: 115:157127
ORIGINAL REFERENCE NO.: 115:26895a,26898a
TITLE: Cinatrin derivatives as phospholipase A2 inhibitors and their manufacture with Circinotrichum falcatisporum
INVENTOR(S): Yoshida, Tadashi; Arita, Hitoshi; Matsumoto, Koichi; Itazaki, Hiroshi; Kawamura, Yoshimi
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 405864	A2	19910102	EP 1990-306872	19900622
EP 405864	A3	19920108		
EP 405864	B1	19950412		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03108490	A	19910508	JP 1990-148007	19900606
AT 121091	T	19950415	AT 1990-306872	19900622
ES 2073529	T3	19950816	ES 1990-306872	19900622
US 5099034	A	19920324	US 1990-544673	19900627
US 5120647	A	19920609	US 1990-617882	19901126
PRIORITY APPLN. INFO.:			JP 1989-170396 A	19890630
			US 1990-544673 A3	19900627

OTHER SOURCE(S): MARPAT 115:157127
GI

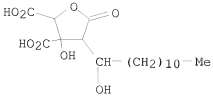


I

AB Cinatrin and its derivs. I (R1, R2, R3 = CO2R4, CO2R5, CO2R6 resp.; R4, R5, R6 = H, lower alkaline, alkaline metal; W, Y, Z = H; W/R3, X/R1, and/or Z/R3 may be combined together to form a lactone, an ester, or salt thereof) are manufacture by fermentation with Circinotrichum falcatisporum with optional hydrolysis and/or esterification. Cinatrins A, B, C2, and C3 were isolated from the fermentation broth of C. falcatisporum. Chemical preparation of their Me esters and seco acid Na salts were also shown. Most chemical modified derivs. were more effective as phospholipase A2 inhibitors.

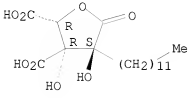
IT 136266-36-9P, Cinatrin C2 136266-37-0P, Cinatrin C3
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)
(manufacture of, with Circinotrichum falcatisporum, as phospholipase A2 inhibitor)

RN 136266-36-9 CAPLUS
CN Pentaric acid, 3-C-carboxy-2-deoxy-2-(1-hydroxydodecyl)-, 1,4-lactone (9CI) (CA INDEX NAME)



RN 136266-37-0 CAPLUS
CN D-Xylaric acid, 3-C-carboxy-2-C-dodecyl-, 1,4-lactone (9CI) (CA INDEX NAME)

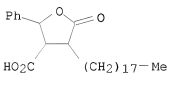
Absolute stereochemistry.



L10 ANSWER 20 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:66804 CAPLUS
DOCUMENT NUMBER: 110:66804
ORIGINAL REFERENCE NO.: 110:10872h,10873a
TITLE: Cyan phenolic coupler containing aromatic ballast group and photographic element containing same
INVENTOR(S): Kilminster, Kenneth Norman; Hoke, David
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 271325	A2	19880615	EP 1987-310812	19871209
EP 271325	A3	19890510		
R: BE, CH, DE, FR, GB, LI, NL				
US 4753871	A	19880628	US 1986-940831	19861212
CA 1298131	C	19920331	CA 1987-530980	19870303
JP 63159848	A	19880702	JP 1987-313174	19871212
JP 07001383	B	19950111		

PRIORITY APPLN. INFO.: US 1986-940831 A 19861212
OTHER SOURCE(S): CASREACT 110:66804
GI For diagram(s), see printed CA Issue.
AB A cyan photog. coupler is described having the formula I [R1 = H, C1-20 alkyl; Q = nonmetallic atoms needed to complete 1-3 rings each having 4-7 atoms; A = NR2, NLR2, CR3R4; R2 = C1-24 alkyl, C3-8 cycloalkyl, C6-24 aryl, C3-8 heterocyclic group having N, O, or S as hetero atom; R3 = R2, halogen; R4 = H, halogen, R2; L = CO, CO2, SO2, CONR5, SO2NR6; R5, R6 = R2, H; Y = ≥1 substituent from halogen, OH, NR7R8, CN, NO2, CO2, SO2, R2; R7, R8 = H, C1-10 alkyl, C6-10 aryl; Z = H or coupling off group]. A photog. element comprising the above coupler produces images with desirable hue without loosing coupler effectiveness. Thus a color film containing II produced an image with λmax 690 nm and half bandwidth 147 nm.
IT 118534-40-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, photog. cyan coupler from)
RN 118534-40-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-octadecyl-5-oxo-2-phenyl- (CA INDEX NAME)

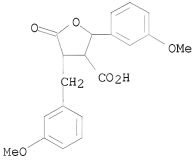


L10 ANSWER 21 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:1066 CAPLUS
DOCUMENT NUMBER: 110:1066
ORIGINAL REFERENCE NO.: 110:183a,186a
TITLE: Molecular interaction of non-steroidal compounds with uterine progesterone receptor (part II)
AUTHOR(S): Agnihotri, Anila; Neelima; Seth, M.; Bhaduri, A. P.; Srivastava, A. K.; Kamboj, V. P.
CORPORATE SOURCE: Div. Endocrinol., Cent. Drug Res. Inst., Lucknow, India
SOURCE: Experimental and Clinical Endocrinology (1988), 91(3), 327-33
CODEN: EXCEDS; ISSN: 0232-7384
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Non-steroidal antiprogestins were evaluated for their receptor binding activity by competitive protein binding assay in rabbit as well as human uterine cytosol in vitro. Of the 42 compds. belonging to 5 different series tested, di-Me ester of monobenzylidene succinic acid, 4-ethoxycarbonyl-3-(m-methoxybenzyl)-5-(m-anisyl)-γ-butyrolactone, and 2-(3-benzyloxybenzyl)-3-(3-acetoxybenzyl)butane-1,4-diol exhibit .apprx.20% inhibition of [3H]progesterone binding to uterine cytosol in both species.

IT 117823-84-4
RL: BIOL (Biological study)
(progesterone binding by receptor of uterine cytosols inhibition by, in human and rabbit, mol. structure in relation to)

RN 117823-84-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(3-methoxyphenyl)-4-[(3-methoxyphenyl)methyl]-5-oxo- (CA INDEX NAME)



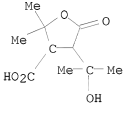
L10 ANSWER 22 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:635736 CAPLUS
DOCUMENT NUMBER: 107:235736
ORIGINAL REFERENCE NO.: 107:37853a,37856a
TITLE: Intermolecular hydrogen-atom abstraction by vinyl radicals derived from hydroxyalkyl radicals and alkynes. An electron spin resonance investigation
AUTHOR(S): Gilbert, Bruce C.; McLay, Neil R.; Parry, David J.
CORPORATE SOURCE: Dep. Chem., Univ. York, Heslington/York, YO1 5DD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1987), (3), 329-36
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The rapid addition of α-hydroxyalkyl radicals •CR1R2OH (R1, R2 = H, Me) to butynedioic acid to give intermediate vinyl radicals (k .apprx. 107 dm3 mol-1 s-1) is followed by intermol. hydrogen-transfer (k .apprx. 106 dm3 mol-1 s-1) from the parent alkanols. The alkenes thus formed also undergo subsequent addition of •CR1R2OH to give radicals which in some cases demonstrate unusual line-broadening effects.

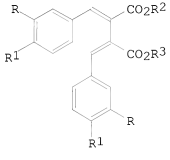
IT 111513-88-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and ESR spectrum of)

RN 111513-88-3 CAPLUS

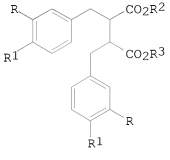
CN 3-Furanyl, 3-carboxytetrahydro-4-(1-hydroxy-1-methylethyl)-2,2-dimethyl-5-oxo- (9CI) (CA INDEX NAME)



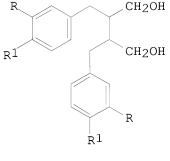
L10 ANSWER 23 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:6070 CAPLUS
DOCUMENT NUMBER: 102:6070
ORIGINAL REFERENCE NO.: 102:1099a,1102a
TITLE: Syntheses of 3,4-bis[(m- or p-substituted-phenyl)methyl]dihydro-2(3H)-furanones and 2,3-bis(m- or p-substituted-benzyl)butane-1,4-diols
AUTHOR(S): Neelima; Bhaduri, A. P.
CORPORATE SOURCE: Div. Med. Chem., Cent. Drug Res. Inst., Lucknow, 226 001, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(3), 209-15
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



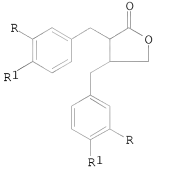
I



II



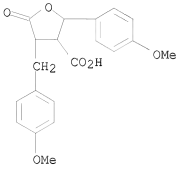
III



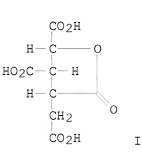
IV

AB Stobbe condensation of appropriately substituted aromatic aldehydes with di-Et or di-Me succinate in the presence of MeONa yields the required starting materials for the syntheses of the title compds. The diacid derivs. I (R = H, MeO, PhCH2O; R1 = H, MeO; R2 = H, R3 = H, Me, Et) so obtained, are catalytically hydrogenated to the esters II (R = H, MeO, HO; R1 = H, MeO; R2 = H; R3 = H, Me, Et), which on esterification give II (R = H, MeO, EtO; R1 = H, MeO; R2 = R3 = Me, Et). LiAlH4 reduction of these diesters furnishes the diols (III), which on oxidn with pyridinium chlorochromate give the desired lactones IV (R = H, MeO, EtO; R1 = H, MeO) in quant. yield.
IT 93578-54-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 93578-54-2 CAPLUS

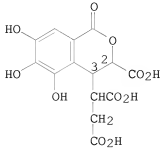
CN 3-Furancarboxylic acid, tetrahydro-2-(4-methoxyphenyl)-4-[(4-methoxyphenyl)methyl]-5-oxo- (CA INDEX NAME)



L10 ANSWER 24 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:34854 CAPLUS
DOCUMENT NUMBER: 98:34854
ORIGINAL REFERENCE NO.: 98:5461a,5464a
TITLE: Phenolic constituents of Quercus valonea
AUTHOR(S): Schilling, G.; Mayer, W.
CORPORATE SOURCE: Org. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Studies in Organic Chemistry (Amsterdam) (1982), Volume Date 1981, 11(Flavonoids Bioflavonoids), 321-4
CODEN: SOCHDQ; ISSN: 0165-3253
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

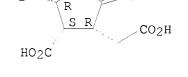


II

AB Phenolic constituents of Q. valonea are discussed. Adipic acid derivative (+)-I, which is obtained by the KMnO4 oxidation of chebulic acid (II) or trilloic acid, was synthesized in order to prove that the substituents at position 2 and 3 in II are in trans arrangement and not cis arrangement as previously claimed (J. C. Jochims, et al). Solution conformation of II is also discussed.

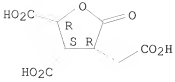
IT 79726-18-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and resolution of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone (9CI) (CA INDEX NAME)

Relative stereochemistry.

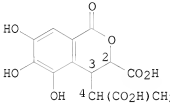


IT 79788-85-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 79788-85-5 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone, (+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.


HO2C
O
O
R
S
R
CO2H
HO2C

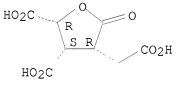
L10 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:603687 CAPLUS
DOCUMENT NUMBER: 95:203687
ORIGINAL REFERENCE NO.: 95:34029a,34032a
TITLE: Relative configuration of chebulic acid
AUTHOR(S): Schilling, Gerhard; Schweiger, Richard; Weis, Guenter; Mayer, Walter; Weiss, Johannes; Siegel, Rolf
CORPORATE SOURCE: Org. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1981), (4), 603-9
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

AB The configuration of chebulic acid (I) was examined by chemical methods, NMR, and x-ray anal.
IT 79726-18-4P 79726-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone (9CI) (CA INDEX NAME)

Relative stereochemistry.

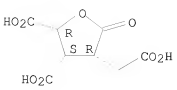


RN 79726-19-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 79788-85-5
CMF C8 H8 O8

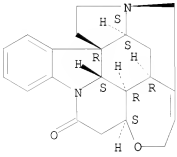
Rotation (+). Absolute stereochemistry unknown.



CM 2

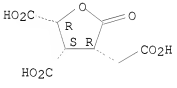
CRN 57-24-9
CMF C21 H22 N2 O2

Absolute stereochemistry. Rotation (-).

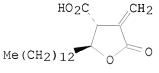


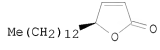
IT 79726-18-4
RL: PROC (Process)
(resolution of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone
(9CI) (CA INDEX NAME)

Relative stereochemistry.



L10 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:523691 CAPLUS
DOCUMENT NUMBER: 85:123691
ORIGINAL REFERENCE NO.: 85:19849a,19852a
TITLE: An efficient and stereospecific total synthesis of DL-protolichesterinic acid
AUTHOR(S): Damon, R. E.; Schlessinger, R. H.
CORPORATE SOURCE: Dep. Chem., Univ. Rochester, Rochester, NY, USA
SOURCE: Tetrahedron Letters (1976), (19), 1561-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:123691
GI


I


II

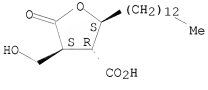
AB The title compound (I), a naturally occurring fungal metabolite possessing antibiotic activity, was stereospecifically prepared in 4 steps from the furan-2-one derivative II (64% overall yield).

IT 60432-64-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 60432-64-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-(hydroxymethyl)-5-oxo-2-tridecyl-, (2R,3S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

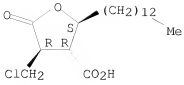


IT 60470-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydrochlorination of)

RN 60470-17-9 CAPLUS

CN 3-Furancarboxylic acid, 4-(chloromethyl)tetrahydro-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

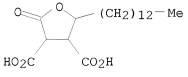

O
O
S
(CH2)12
Me
R
R
ClCH2
CO2H

L10 ANSWER 27 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:424999 CAPLUS
DOCUMENT NUMBER: 81:24999
ORIGINAL REFERENCE NO.: 81:4041a,4044a
TITLE: Carboxylation of γ-butyrolactones with methyl methoxymagnesium carbonate. New synthesis of DL-protolichesterinic acid
AUTHOR(S): Martin, Jack; Watts, Paul C.; Johnson, Francis
CORPORATE SOURCE: East. Res. Lab., Dow Chem. U.S.A., Wayland, MA, USA
SOURCE: Journal of Organic Chemistry (1974), 39(12), 1676-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 81:24999

AB The carboxylation of γ-lactones at the α position is, in most cases, easily accomplished by means of Stiles' reagent (methyl methoxymagnesium carbonate). This combined with a simplified decarboxylative methylenation procedure, namely treatment of the α-carboxylactones with a mixture of formaldehyde and diethylamine, usually in a buffered acidic medium, affords a relatively simple method of synthesizing α-methylenelactones. These methods have been used in a new synthesis of dl-protolichesterinic acid.

IT 51175-46-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(decarboxylation-methylenation of)

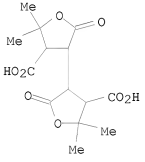
RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



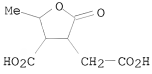
L10 ANSWER 28 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:442880 CAPLUS
DOCUMENT NUMBER: 77:42880
ORIGINAL REFERENCE NO.: 77:7051a,7054a
TITLE: Chromatographic analysis of mixtures of aliphatic dicarboxylic acids and lactones
AUTHOR(S): Kucera, J.
CORPORATE SOURCE: Inst. Nucl. Res., Rez/Prague, Czech.
SOURCE: Fette, Seifen, Anstrichmittel (1972), 74(3), 143-50
CODEN: FSASAX; ISSN: 0015-038X
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Aliphatic dicarboxylic acids and lactones were separated and identified by 8.5:1.5 96% EtOH-NH4OH, 3:1 Me2CO-0.5N NH4OAc, or 3:1 Me2CO-0.5N HOAc solvent system and by thin-layer chromatog. on silica gel G with 8:1.6:0.4 PrOH-H2O-NH4OH developing solvent. Hydroxy acids and cis- and trans-isomers of unsatd. acids can be separated Rf data for 37 compds. are given. Spots were visualized by spraying with 5% AgNO3 in 10% NH3 solution and heating at 110° or by spraying with 0.5% KMnO4 in 2.5% H2SO4 (for unsatd. acids).

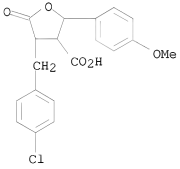
IT 38840-99-2
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of)
RN 38840-99-2 CAPLUS
CN [3,3'-Bifuran]-4,4'-dicarboxylic acid, octahydro-5,5,5',5'-tetramethyl-2,2'-dioxo- (CA INDEX NAME)



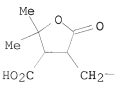
L10 ANSWER 29 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:13122 CAPLUS
DOCUMENT NUMBER: 74:13122
ORIGINAL REFERENCE NO.: 74:2117a,2120a
TITLE: Bitter principle of Jasminum primulinum. II. Structure and reactions of jasminim
AUTHOR(S): Kamikawa, Tadao; Inoue, Ken; Kubota, Tokuo; Woods, M. C.
CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, Japan
SOURCE: Tetrahedron (1970), 26(19), 4561-87
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The structure of jasminim (I, R = β-D-glucosyl), a bitter principle of J. primulinum (jasmine) based on a study of the chemical and phys. properties was confirmed by x-ray anal.
IT 30203-69-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30203-69-1 CAPLUS
CN 3-Furanacetic acid, 4-carboxytetrahydro-5-methyl-2-oxo- (CA INDEX NAME)



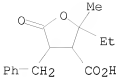
L10 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1968:506156 CAPLUS
DOCUMENT NUMBER: 69:106156
ORIGINAL REFERENCE NO.: 69:19863a,19866a
TITLE: Lactone carboxylic acids. V. Preparation of a lignan skeleton
AUTHOR(S): Takeda, Akira; Torii, Sigeru
CORPORATE SOURCE: Okayama Univ., Okayama, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1968), 41(6), 1468-71
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The treatment of I (R = H, R1 = CO2Et) with 4-ClC6H4CH2Cl and EtONa gave I (R = CH2C6H4Cl-4, R1 = CO2H) and 4-MeOC6H4CH:C(CO2Et)CH(CO2Et)CH2C6H4Cl-4.
IT 20375-12-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20375-12-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[(4-chlorophenyl)methyl]tetrahydro-2-(4-methoxyphenyl)-5-oxo- (CA INDEX NAME)



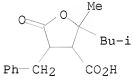
L10 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1967:481911 CAPLUS
DOCUMENT NUMBER: 67:81911
ORIGINAL REFERENCE NO.: 67:15419a,15422a
TITLE: Lactone carboxylic acids. I. Synthesis of α,γ-substituted paraconic acids
AUTHOR(S): Takeda, Akira; Torii, Sigeru
CORPORATE SOURCE: Okayama Univ., Okayama, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1967), 40(5), 1261-3
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:81911
GI For diagram(s), see printed CA Issue.
AB Benzylation, but not alkylation or alkenylation, of α,β-dicarbethoxy-γ, γ-dialkylbutyrolactones (I, R = Et, R2 = H, R3 = CO2Et) (II) with organic chlorides in the presence of NaOMe proceeds in the α-position in good yields. Thus, II (from the condensation of Et β,β-dialkylglycidates with malonates in alc. in the presence of NaOMe) is condensed with benzyl chlorides in alc. NaOMe to give the following I (R = H, R3 = CO2Et) (III) (R1, R2, % yield, b.p., and m.p. given): Me, PhCH2, 85, b3 183-6°, 54°; Et, PhCH2, 57, b2.5 180°, -; iso-Bu, PhCH2, 51, b1 175°, -; iso-Am, PhCH2, 58, b2 162°, -; Me, p-ClC6H4CH2, 56, b2 196°, 65°; Me, 3,4-methylenedioxybenzyl, 70, b2 215°, -; Me, allyl, 23, b2 142°, -; Me, methallyl, 1, b2 138-42°, -; Me, Bu, 1-2, b11 125-30°, -. Hydrolysis designed to affect only the carbethoxy group of II was carried out with NaOH in 99% alc. 7 hrs. at room temperature to give the following I (R = Et, R2 = H) (IV) (R1, R3, % yield, b2.5, and m.p. given): Me, PhCH2, 63, 156°, -; Et, PhCH2, 54, 180°, -; Me, p-ClC6H4CH2, 72, -, 82°; Me, 3,4-methylenedioxybenzyl, 73, -, 92°; Me, allyl, 43, 122-6°, -. Refluxing IV with excess NaOH 6 hrs. splits the β-carbethoxy group to give the following I (R = R2 = H) (V) (R1, R3, % yield, and m.p. given): Me, PhCH2, 55, 179°; Me, p-ClC6H4CH2 (Va), 62, 208°; Me, 3,4-methylenedioxybenzyl, 32, 75°. More prolonged hydrolysis cleaves the lactone ring as well. V can also be obtained in 60-90% yields from either III or IV by HBr-catalyzed hydrolysis in refluxing AcOH; however, Va could not be prepared by this route.
IT 15312-93-3P 15312-94-4P 15312-95-5P
15312-96-6P 15312-97-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15312-93-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2,2-dimethyl-5-oxo-4-(phenylmethyl)- (CA INDEX NAME)



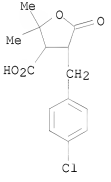
RN 15312-94-4 CAPLUS
CN 3-Furancarboxylic acid, 2-ethyltetrahydro-2-methyl-5-oxo-4-(phenylmethyl)- (CA INDEX NAME)



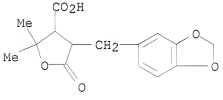
RN 15312-95-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-methyl-2-(2-methylpropyl)-5-oxo-4-(phenylmethyl)- (CA INDEX NAME)



RN 15312-96-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[(4-chlorophenyl)methyl]tetrahydro-2,2-dimethyl-5-oxo- (CA INDEX NAME)



RN 15312-97-7 CAPLUS
CN 3-Furancarboxylic acid, 4-(1,3-benzodioxol-5-ylmethyl)tetrahydro-2,2-dimethyl-5-oxo- (CA INDEX NAME)

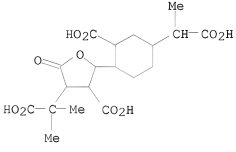


L10 ANSWER 32 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:412495 CAPLUS
DOCUMENT NUMBER: 65:12495
ORIGINAL REFERENCE NO.: 65:2306b-c
TITLE: Structure of two solanone precursors from tobacco
AUTHOR(S): Kinzer, Glenn W.; Page, Thomas F., Jr.; Johnson, Robert R.
CORPORATE SOURCE: Org. Chem. Div., Battelle Mem. Inst., Columbus, OH
SOURCE: Journal of Organic Chemistry (1966), 31(6), 1797-1800
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

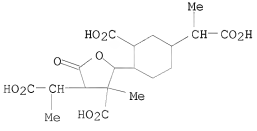
AB Two acyclic diterpenoid precursors of solanone have been isolated from tobacco and identified as diastereoisomers of 6,8-dihydroxy-11-isopropyl-4,8-dimethyl-14-oxo-4,9-pentadecadienoic acid.

IT 6619-91-6P, 3-Furanacetic acid, 4-carboxy-5-[2-carboxy-4-(1-carboxyethyl)-cyclohexyl]tetrahydro-α,α-dimethyl-2-oxo- 856818-96-7P, 2,3,4-Pentanetricarboxylic acid, 1-[2-carboxy-4-(1-carboxyethyl)cyclohexyl]-1-hydroxy-2-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

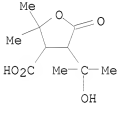
RN 6619-91-6 CAPLUS
CN 3-Furanacetic acid, 4-carboxy-5-[2-carboxy-4-(1-carboxyethyl)cyclohexyl]tetrahydro-α,α-dimethyl-2-oxo- (CA INDEX NAME)



RN 856818-96-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



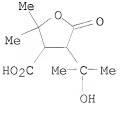
L10 ANSWER 33 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:59448 CAPLUS
DOCUMENT NUMBER: 55:59448
ORIGINAL REFERENCE NO.: 55:11386g-h
TITLE: Photosensitized addition of isopropyl alcohol to acetylenedicarboxylic acid
AUTHOR(S): Schenck, Gunther O.; Steinmetz, Reinhard
CORPORATE SOURCE: Max-Planck-Inst., Mulheim-Ruhr, Germany
SOURCE: Naturwissenschaften (1960), 47, 514-15
CODEN: NATWAY; ISSN: 0028-1042
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB In the presence of Ph2CO (I), which acted as a photosensitizer, high-energy radiation effected the radical addition of iso-PrOH (II) to (HO2CC.tplbond.)2 to produce 23.6% dilactone, 4,4,8,8-tetramethyl-3,7-dioxa-2,6-dioxo[3.3.0]bicyclooctane (III), m. 110°, and 36.9% 1-(2-hydroxyisopropyl)-2-carboxy-3,3-dimethyl-4-oxacyclopentan-5-one (IV), m. 155°. III and IV were also prepared via the radical addition of II to terebilenic acid, O.CO.CH:C(CO2H).CMe2, in the presence of I. I was believed to be dissociated by high-energy radiation into semi-benzopinacol radicals, the active agents. Treatment of III with strong base and of IV with H2SO4 yielded 1-isopropyl-2-carboxy-3,3-dimethyl-4-oxa-1-cyclopentene-5-one, m. 125°. Treatment of IV with hot aqueous NaOH yielded terebic acid and Me2CO.
IT 109841-10-3
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109841-10-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-hydroxy-1-methylethyl)-2,2-dimethyl-5-oxo- (CA INDEX NAME)



L10 ANSWER 34 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:59447 CAPLUS
DOCUMENT NUMBER: 55:59447
ORIGINAL REFERENCE NO.: 55:11386c-g
TITLE: Studies on furfural. XX. The mixed heterogenous Canizzaro reaction between 2-furaldehyde and formaldehyde. 2. The role of hydration equilibria
AUTHOR(S): Paucescu, Stelian D.
CORPORATE SOURCE: Acad. R.P.R., Bucharest, Rom.
SOURCE: Studii si Cercetari de Chimie (1960), 8, 465-74
CODEN: SCECA2; ISSN: 0039-3908
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 55, 8376c. The mixed heterogenous Canizzaro reaction between 2-furaldehyde and HCHO was studied to determine the effect of the hydration equilibria on the reaction. In 37% HCHO the following hydration equilibrium were determined between methylene glycol, di-, and trimethylene glycol by ultrasonics, infrared and ultraviolet spectra, and magnetic susceptibility: HCHO .dblharw. H2O + CH2(OH)2 .dblharw. H2O + HOCH2OCH2OH .dblharw. H2O + HOCH2OCH2OCH2OH, 0.01% HCHO, 3-4% CH2(OH)2, and the remainder 95.89-96.89% di- and trimethylene glycol, the equilibrium varying with temperature and concentration of HCHO. On dilution, the di- and trimethylene glycol depolymerized with an energy consumption of 17.4 kcal./mole. The MeOH also present as stabilizer determined parallely a solvation equilibrium to form together with the glycol a dynamic solvation-hydration equilibrium which favored the 1st equilibrium, limited by the amount of MeOH in the solution Increase of the MeOH concentration from 0 to 26.85% reduced gradually the reaction rate of HCHO in the self-Canizzaro while the activation energy increased from 22.32 to 26.24 kcal./mole. This activation energy and the solvating tendency of the aldehyde increased with the dielectric constant of the medium. Since the activation energy of 2-furaldehyde in the self-Canizzaro reaction was 11.25 kcal./mole, it was clear that it would be reduced to furfuryl alc. while the HCHO would be oxidized to HCO2H. Since the di- and trimethylene glycols did not participate in the reaction, their slow and gradual depolymerization to supply methylene glycol was liable to react by restraining the HCHO reduction, favoring 2-furaldehyde reduction Based on theoretical calcns., the maximum obtainable conversion yield of 2-furaldehyde to furfuryl alc. was 92.98%. 11 references.

IT 109841-10-3
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109841-10-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-hydroxy-1-methylethyl)-2,2-dimethyl-5-oxo- (CA INDEX NAME)



L10 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:59200 CAPLUS
DOCUMENT NUMBER: 55:59200
ORIGINAL REFERENCE NO.: 55:11310c-d
TITLE: Aliphatic saturated esters of dicarboxylic acids
INVENTOR(S): Illing, Gerhard; v. Kutepow, Nikolaus
PATENT ASSIGNEE(S): Badische Anilin- & Soda-Fabrik Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

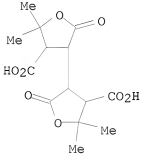
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1070613		19591210	DE	

AB 1,4-Butanediol or butyrolactone condenses with CO in the presence of Ni, iodine, Bi, and H2O at 240°/250-70 atmospheric and the carbonylation product is esterified with alcs., e.g. 2-ethylhexanol, to give esters of C6 dicarboxylic acids, suitable for use as plasticizers. Cf. Reppe, et al., CA 48, 11311b.

IT 38840-99-2P, [3,3'-Bifuran]-4,4'-dicarboxylic acid, octahydro-5,5,5',5'-tetramethyl-2,2'-dioxo-
RL: PREP (Preparation)
(preparation of)

RN 38840-99-2 CAPLUS

CN [3,3'-Bifuran]-4,4'-dicarboxylic acid, octahydro-5,5,5',5'-tetramethyl-2,2'-dioxo- (CA INDEX NAME)



L10 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:59199 CAPLUS
DOCUMENT NUMBER: 55:59199
ORIGINAL REFERENCE NO.: 55:11310a-c
TITLE: Alkyl-substituted butyrolactones and their carboxylic acids
INVENTOR(S): Schenck, Otto
PATENT ASSIGNEE(S): Farbwerke Hoechst AG
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1063142		19590813	DE 1956-F21882	19561208

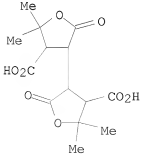
OTHER SOURCE(S): CASREACT 55:59199

AB Mixts. of α,β-unsatd. aliphatic mono- or dicarboxylic acids and primary or secondary aliphatic alcs. were irradiated with ultraviolet light in the presence of photosensitizing agents to give the title compds., useful as intermediates in the manufacture of pharmaceuticals. Thus, 10 g. fumaric acid (I) and 4 g. Ph_2CO (II) in 150 cc. iso-PrOH was irradiated 4 hrs. with stirring, the solution concentrated, the residue extracted with hot H_2O (60°), the extract cooled, the unreacted I filtered off, the filtrate acidified with H_2SO_4, and concentrated to half volume to give γ,γ-dimethylbutyrolactone-β-carboxylic acid, m. 175°. Alternatively, maleic acid (III) could be irradiated instead of I. Similarly, III treated with $MeCH_2CHMeOH$ in the presence of II gave γ-methyl-γ-ethylbutyrolactone-β-carboxylic acid, m. 130° (H_2O), besides (apparently) γ,γ-diphenylbutyrolactone-β-carboxylic acid, m. 80-110°. $MeCH{:}CHCO_2H$ treated with iso-PrOH in the presence of Me_2CO gave α,α'-bis(γ,γ-dimethyl-β-methyl-butyrolactone), m. 121°, besides γ,γ-dimethylbutyrolactone, m. 5-6°, b1-2 71-2°. I treated with iso-PrOH in the presence of Me_2CO gave α,α'-bis(γ,γ-dimethylbutyrolactone-β-carboxylic acid).

IT 38840-99-2P, [3,3'-Bifuran]-4,4'-dicarboxylic acid, octahydro-5,5,5',5'-tetramethyl-2,2'-dioxo-
RL: PREP (Preparation)
(preparation of)

RN 38840-99-2 CAPLUS

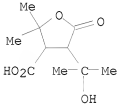
CN [3,3'-Bifuran]-4,4'-dicarboxylic acid, octahydro-5,5,5',5'-tetramethyl-2,2'-dioxo- (CA INDEX NAME)



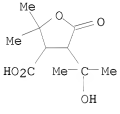
L10 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:37680 CAPLUS
DOCUMENT NUMBER: 55:37680
ORIGINAL REFERENCE NO.: 55:7283a-b
TITLE: Organosilyl dithiocarbamates
AUTHOR(S): Breederveld, H.
CORPORATE SOURCE: Univ. Eindhoven, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1960), 79, 1126
CODEN: RTCPB4; ISSN: 0370-7539
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dialkylaminosilanes react with CS2 at room temperature to give the corresponding silyldialkyldithiocarbamates, Me3SiNEt2 + CS2 → Me3SiSCSNEt2 (I). The structure of I is established by its synthesis. Heating the silyldialkyldithiocarbamates at 100° reverses the reaction to give CS2.

IT 109841-10-3
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109841-10-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-hydroxy-1-methylethyl)-2,2-dimethyl-5-oxo- (CA INDEX NAME)



L10 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:37679 CAPLUS
DOCUMENT NUMBER: 55:37679
ORIGINAL REFERENCE NO.: 55:7282g-i,7283a
TITLE: Photochemical addition of alcohols to α,β-acetylenic acids
AUTHOR(S): Pfau, Michel; Dulou, Raymond; Vilkas, Michel
CORPORATE SOURCE: Ecole normale super., Paris
SOURCE: Compt. rend. (1960), 251, 2188-90
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Photochem. addition of 1 or 2 equivs. of iso-PrOH (I) to triple bonds activated by a carboxyl group was described. Thus, 12.1 g. propiolic acid and 4 g. Ph2CO in 400 cc. I was irradiated 24 hrs. at reflux temperature, the solvent evaporated and the residue taken up in ether, washed with Na2CO3 solution and distilled, giving 6.7 g. 4-methyl-2-pentene-2-olide-1,4, b0.5 30-1°, n21D 1.4423, d20 1.022. Acetylenedicarboxylic acid (17 g.), 4 g. Ph2CO, and 400 cc. I were irradiated 60 hrs. at 35°, the solvent was evaporated and the residue taken up in ether. Filtration gave 3.5 g. dilactone OC.O.CMe2.CH.CH.CMe2.O.CO (II). The filtrate was extracted with Na2CO3 solution and 4.3 g. of II isolated from the neutral fraction, m. 120-4° (benzene-petr. ether). The aqueous layer was acidified with H2SO4, extracted with ether and evaporated, the residue was added to benzene and the solution heated to reflux. Cooling gave 4 g. β-(1-hydroxy-1-methylethyl)terebic acid, m. 154-5° (H2O).
IT 109841-10-3
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109841-10-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-(1-hydroxy-1-methylethyl)-2,2-dimethyl-5-oxo- (CA INDEX NAME)

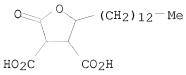


L10 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:113135 CAPLUS
DOCUMENT NUMBER: 52:113135
ORIGINAL REFERENCE NO.: 52:19935a-g
TITLE: Condensation of aldehydes with esters of oxaloglycolic acid and oxalacetylglycolic acid
AUTHOR(S): Elkik, Elias
SOURCE: J. recherches centre natl. recherche sci. labs. Bellevue (Paris) (1958), No. 40, 176-96
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

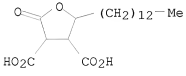
AB The preparation is given, by a modified method, of glycolic acid and also a synthesis of oxaloglycolic and oxalacetylglycolic acid esters and an infrared spectrometric study of their structures, especially of their behavior in alkaline medium. Condensation of these esters with HCHO and BzH failed to give the expected products, either in alkaline or a buffered acid medium. The ultimate objective (the conversion of oxoparaconic esters into the ene-diol structure of ascorbic acid) was not accomplished. Glycolic acid, prepared by the hydrolysis of ClCH2CO2H by BaCO3 in an autoclave for 5 hrs. with addition of 10% H2SO4 and evaporation in vacuo at a temperature lower than 70°, was esterified by EtOH and the Et glycolate converted to Et acetylglycolate, b. 84°, by AcCl. Similarly, Et benzoylglycolate, b12-14 160-5°, was obtained. Condensation of Et oxalate with either acylated ester, gave Et oxaloglycolate (I), m. 72-4°, a mixture of 2 isomers, the enediol (Ia), m. 68°, and ketol (Ib), m. 165-6°. The 2 forms were separated and studied by infrared spectroscopy, and compared with prepns. made by Fenton (C.A. 7, 332). Both Ia and Ib were unstable in strong or weak alkaline solution decomposing by hydrolysis and decarboxylation. Et oxalacetylglycolate (II), m. 93-6°, was separated into 2 isomers, the keto form, m. 100-1°, and the isomeric enediol, m. 93-4°. The mode of decomposition of these isomers by alkali at different pH with suggested mechanism was discussed. Condensations of I with HCHO or BzH in alkaline yielded only degradation products; in buffered acid medium (94 g. I in 500 cc. of aqueous solution containing 30 g. AcOH, 68 g. crystalline AcONa, and 50 cc. 30% HCHO, shaken for 5 hrs. at -10°) the product was Et methylenebisoxalacetate-H2O, m. 115-16°, identified by the dinitrophenylhydrozone, m. 158-9°. Heat converted the ester into anhydrous form, m. 83°. Condensation of II with HCHO in alkaline medium (12.5 g. II in 25 cc. H2O was treated with 6 cc. 30% HCHO and 21 g. K2CO3, shaken 6 hrs. acidified with 20 cc. 50% HCl, extracted with Et2O, washed, dried over Na2SO4, recrystd. from H2O) yielded Et oxobutyrolactonecarboxylic acid, [m. 108°; enolate, m. 255-6° (decomposition)], relatively stable at pH <9. The normal condensation product (α-oxo-β-acetoxy-β-carboxyethyl-γ-butyrolactone) was not isolated, but pyruvic acid, a product of decomposition of the latter, was isolated and characterized by its phenylhydrazone, m. 190-2°. Condensation of II with BzH in alkaline medium (12.5 g. II in 25 cc. absolute EtOH was treated with 5.4 g. BzH then 15 cc. NHEt2, stirred 6 hrs. and kept cold overnight, 50% HCl added to pH 1, extracted with Et2O, washed, recrystd. from EtOH) yielded α-oxo-β,γ-diphenyl-γ-butyrolactone, m. 212-14°, identical with that isolated by Erlenmeyer [Ber. 27, 2225 (1894)]. A mechanism was suggested showing that the first lactone formed split off phenylpyruvic acid, then was converted into the above lactone. Condensation of II in acid medium, using the method described for I, was unsuccessful; recovery of 7 g. of the original 12.5 g. of ester and only 2 g. of a viscous liquid resulted. At pH 5-6 in buffered solution condensation is not effected.

IT 5117-5-46-3 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)



L10 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:56698 CAPLUS
DOCUMENT NUMBER: 51:56698
ORIGINAL REFERENCE NO.: 51:10470b-i,10471a-i,10472a
TITLE: Synthesis of dl-asarinin and dl-sesamin
AUTHOR(S): v. Bruchhausen, Friedrich; Lingner, Klaus
CORPORATE SOURCE: Tech. Hochschule, Braunschweig, Germany
SOURCE: Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1957), 290, 1-16
CODEN: APBDAJ; ISSN: 0376-0367
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:56698

AB dl-Sesamin (I), 2,6-bis(3,4-methylenedioxyphenyl)-cis-3,7-dioxabicyclo[3,3,0]octane, and its diastereoisomer dl-asarinin (II) have recently been synthesized (cf. Beroza and Schechter, C. A. 50, 13859a; Freudenberg and Fischer, C.A. 51, 2719g) by dehydration and double ring closure of 1,4-bis(3,4-methylenedioxyphenyl)-2,3-bis(hydroxymethyl)-1,4-butanediol, obtained by LiAlH4 reduction of the oily form of di-Et 2,3-bis(3,4-methylenedioxybenzoyl)succinate (III) (cf. v. Bruchhausen and Gerhard, C.A. 33, 5391⁴). Synthesis of I and II by ring closure through the Hofmann degradation of the diol-diammonium base of a tetrol with suitable configuration has been investigated since the resolution of the intermediate diol-diamine might afford the optically active dioxabicyclooctanes. As a model substance, the "asarinin half-molecule," 2-(methylenedioxyphenyl)tetrahydrofuran (IV) was synthesized. EtMgBr (from 3.5 g. Mg and 15 g. EtBr in 500 ml. absolute Et2O) treated dropwise with 9 g. HC.tplbond.CCH2NMe2 in Et2O, the mixture refluxed 20 min. and treated dropwise with 11 g. piperonal, the mixture refluxed 5 hrs., decomposed with NH4OH and ice, the Et2O layer shaken with dilute HCl, the acid extract made alkaline with NH4OH and extracted with Et2O and the washed and dried extract evaporated gave 10 g. hydroxypiperonylpropargyldimethylamine, reduced 8 hrs. in 100 ml. 50% AcOH with 0.5 g. prereduced PtO2, filtered and worked up to give 8 g. 3-(α-hydroxypiperonyl)propyldimethylamine; MeI derivative (V), m. 208-11°. V (5 g.) in 300 ml. hot H2O digested with Ag2O (from 5 g. AgNO3), filtered and the filtrate concentrated to 20 ml., the concentrate treated with 20 g. KOH, the mixture refluxed at 140-50°, the cooled product extracted with Et2O, the extract evaporated and the residue distilled gave 2.2 g. IV, b1.5 130°, stable to oxidation with KMnO4. The furan ring closure to the model compound through Hofmann degradation was therefore feasible. As possible intermediates for bis(α-hydroxypiperonyl)bis(dimethylamino)butane (VI), the preparation of di-Et dipiperonylfumarate (VII), di-Et bis(a-hydroxypiperonyl)succinate (VIII) and the corresponding lactone (VIIIa) was investigated. III (2 g.) kept several days with 30 ml. 65% aqueous NHMe2, the mixture filtered and the crystalline product recrystd. from AcOH gave the known dipiperonoylethane, m. 216-18°, instead of the expected VI. III (9.4 g.) refluxed 15 min. with 0.9 g. K in 200 cc. absolute alc., the deep-yellow solution cooled, diluted with 200 ml. H2O and acidified with HCl, filtered and the residue crystallized from alc. yielded 4.8 g. Et dipiperonoylsuccinate enol lactone (VIIIb), m. 151-3°, not converted by reduction to the required VIIIa. II (30 g.) in 800 ml. Et2O treated with 10 g. Al-Hg, decomposed after cessation of H evolution by gradual addition of H2O, kept 24 hrs. and the Et2O layer filtered off, dried, and evaporated, part of the 25 g. oily residue fractionally distilled, the oily product chromatographed over Al2O3 and eluted with C6H6 gave di-Et piperonyl(α-hydroxypiperonyl)succinate, saponified to piperonyl(α-hydroxypiperonyl)succinic acid monolactone, m. 242-4°. The oily residue (10 g.) in 50 ml. alc. treated 15 hrs. at room temperature with 10 g. 50% KOH, the mixture diluted with H2O and extracted with

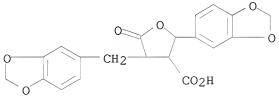
Et2O, the extract evaporated and the residue recrystd. from C6H6-petr. ether gave
di-Et piperonyl(α-hydroxypiperonyl)succinate, m. 96-101°, saponified to an acid, m. 215°, not further investigated since the reduction had failed to give the required VIII. The dehydrogenation of III to di-Et dipiperonylfumarate (IX) was investigated. III (65 g.) in 300 ml. AcOH and 300 ml. dioxane heated 30 hrs. on a steam bath with 130 g. Hg(OAc)2, the cooled mixture filtered, the precipitate washed and dried gave 68
g. Hg(OAc). The concentrated filtrate taken up in Et2O, shaken with ice and concentrated NaOH to alkaline reaction, the Et2O layer separated and combined with the
Et2O washings of the residual layer, the extract evaporated, the oily residue taken up in 600 ml. hot alc., cooled and treated with 30 drops of 25% NH4OH yielded 21 g. IX, m. 144-6°, reduced in AcOH in the presence of prereduced PtO2 to III, m. 162°, and lactonized by warming in absolute alc. with NaOEt to VIIIb. IX (1 g.) refluxed 30 min. with 0.4 g. KOH in 40 ml. alc., the mixture diluted with H2O and acidified with dilute H2SO4, filtered and the product crystallized from alc. gave dipiperonoylfumaric acid, m. 254-6° (decomposition). Saponification with concentrated alc. KOH for an extended
period gave, in addition to the acid, the yellow neutral dipiperonoylethane, m. 262-4° (from dioxane). Since attempts to convert IX into the required dipiperonoylfumaric acid bis(dimethylamide) failed it was decided to begin with intermediates already containing the N functional group such as the known ω-cyanoacetopiperone (X), piperonoylacetamide (Xa), and piperonoylacetodimethylamide (Xb) which on dimerization, reduction and, if necessary, methylation might lead to the required VI. Et piperonylate (24 g.) treated 30 min. with 5 g. MeCN, 30 g. C6H6, and 15 g. 50% NaNH in C6H6, the yellow mixture poured into ice H2O and acidified with HCl, filtered, and the product crystallized from alc. gave 16 g. X, m. 133-5°. X (20 g.) in 20 ml. absolute alc. and 150 ml. dioxane saturated at 0° with dry HCl, refrigerated 10 hrs., and seeded gave 22 g. piperonoylacetimido Et ether-HCl (XI), m. 145°, converted by heating 5 min. over 150° and crystallizing the crude melt from alc. to 63% Xa, m. 150-1°, yielding mixts. on attempts at dimerization with NaOEt and iodine due to the presence of the reactive unsubstituted NH2 group. XI (2 g.) in 30 ml. absolute alc. treated several days with excess NHMe2 in absolute alc., the mixture evaporated in vacuo, and the residue recrystd.
from Me2CO containing absolute alc. gave piperonoylacetodimethylamidinium chloride, m. 169°, neutralized in aqueous solution with NaOH to the free base, m. 186-8°, hydrolyzed by dilute alc. NaOH or NaOAc to piperonylic acid and unaffected by refluxing 5 hrs. with 8% H2SO4. Another way for the preparation of Xb was investigated. AcCl (66 g.) in C6H6 added dropwise to 320 g. 23% NHMe2 in C6H6 at 0°, the mixture kept at room temperature several hrs., filtered, the residual NH2Me2Cl washed with C6H6,
the C6H6 exts. distilled and the residue fractionated gave 60.5 g. AcNMe2, b. 160-70°. The amide (18 g.) and 42 g. Et piperonylate in 250 ml. C6H6 treated with 40 g. 50% NaNH2 in C6H6, the mixture heated 5 hrs. on a steam bath, poured into ice H2O and acidified, filtered and the residue washed thoroughly with C6H6, the filtrate separated and the C6H6 phase dried and evaporated, the oily residue fractionated and the fraction, b0.5 180°, crystallized from C6H6 gave a crude product, m. 60-5°, purified by extraction with Et2O and recrystn. from CHCl3-Et2O or C6H6-petr. ether to pure Xb, m. 87-8°, red-violet coloration with FeCl3. Xb (2.4 g.) in 150 ml. C6H6 treated with 20 ml. 0.54M PhLi in Et2O and 1.2 g. iodine in 50 ml. C6H6, the mixture warmed 1 hr. on a steam bath, the supernatant liquid decanted and the residue taken up in CHCl3, both organic solns. washed with aqueous Na2S2O3 and H2O, the combined dried solns. evaporated,

the residue taken up in C6H6 and kept, the crystalline product (1.7 g.) chromatographed over Al2O3 from C6H6, and the fraction on evaporation recrystd. from Et2O gave dipiperonoylsuccinic acid bis(dimethylamide) (XII), m. 208-11°, FeCl3 reaction neg., rapidly reducing triphenyltetrazolium chloride. The mother liquors yielded 0.7 g. oil (XIIa), probably a mixture of tautomeric forms and by-products. XII (5 g.) in 150 ml. dioxane added dropwise to 1.5 g. LiAlH in 500 ml. boiling Et2O, the mixture refluxed 4 hrs., the excess LiAlH4 decomposed with H2O and 15 ml. saturated NH4Cl, the mixture shaken, settled and the organic layer separated, washed with dilute H2SO4, the aqueous acid solution made alkaline and extracted with Et2O, and the dried extract evaporated yielded 4 g. bright-yellow oily diastereomeric VI. Reduction of XIIa gave an amorphous basic mixture VI (3.5 g.) in 50 ml. tetrahydrofuran refluxed 2 hrs. with 3.5 g. MeI, the cooled mixture decanted and the oily residue taken up in alc. and a min. of hot H2O, and the crystalline product (1 g.) recrystd. from alc. gave VI di-MeI derivative (XIII), m. 269-71°. Similarly the amorphous mixture produced an oily methiodide (XIIIa). XIII (1 g.) in 200 cc. H2O digested with Ag2O (from 1 g. AgNO3), filtered, the filtrate evaporated and the residue heated 20 min. at 160-70°, the cooled degradation product extracted with Et2O, the extract evaporated and the residue crystallized from alc. gave 0.1 g. I, m. 123°, stable to KMnO4 oxidation and identical with authentic I in infrared and ultraviolet spectra. Crystallization of the degradation product from XIIIa gave a small yield of II, m. 133°, with ultraviolet spectrum identical with that of I. This synthesis of I by Hofmann degradative double ring closure gives only 20% yield and an indefinite yield of II.

IT 111034-18-5P, Succinic acid, 2-(α-hydroxypiperonyl)-3-piperonyl-, lactone
RL: PREP (Preparation)
(preparation of)

RN 111034-18-5 CAPLUS

CN 3-Furancarboxylic acid, 2-(1,3-benzodioxol-5-yl)-4-(1,3-benzodioxol-5-ylmethyl)tetrahydro-5-oxo- (CA INDEX NAME)



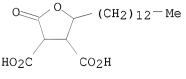
L10 ANSWER 41 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:34629 CAPLUS
DOCUMENT NUMBER: 51:34629
ORIGINAL REFERENCE NO.: 51:6517c-i,6518a-d
TITLE: Preparation and properties of the isomeric forms of α-amino- and α,ε-diaminopimelic acid
AUTHOR(S): Wade, Roy; Birnbaum, Sanford M.; Winitz, Milton; Koegel, Robert J.; Greenstein, Jesse P.
CORPORATE SOURCE: Natl. Insts. of Health, Bethesda, MD
SOURCE: Journal of the American Chemical Society (1957), 79, 648-52
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:34629
AB CH2(CH2CH2CO2Et)2 cyclized by the method of Dobson, et al., (C.A. 4, 1028) yielded 76% α-carbethoxycyclohexanone (I), b0.4 70-2°. I coupled with PhN2Cl by the method of Jackson and Manske (C.A. 25, 514) gave 60% Et H α-oxopimelate phenylhydrazone, m. 141-2° (decomposition), which saponified with 1.1N NaOH in 50% aqueous dioxane gave HO2C(CH2)4C(:NNHPh)CO2H (II), prisms, m. 141-3° (decomposition) (from EtOAc-petr. ether). II (10 g.) refluxed 6 hrs. with 15 g. Zn dust and 150 cc. 75% AcOH, filtered, and evaporated, the residue dissolved in 50 cc. H2O, treated 3 hrs. with H2S; filtered hot, and evaporated to dryness, and the crystalline residue shaken with a little EtOH and filtered gave HO2C(CH2)4CH(NH2)CO2H (III), plates, m. 216° (decomposition) (from aqueous EtOH). III (3.5 g.) in 25 cc. 2N NaOH treated at 5° with 2.2 cc. Ac2O and 20 cc. 2N NaOH in alternate portions with shaking and cooling, the mixture kept 1 hr. at room temperature, acidified to about pH 1.7 with 4N HCl and evaporated at 40° in vacuo, the residue diluted with 20 cc. H2O, the evaporation repeated, the crsyt. residue extracted with hot Me2CO, and the extract filtered, concentrated, diluted with Et2O to incipient turbidity, scratched, and filtered yielded 2.5 g. N-Ac derivative (IV) of III, m. 111-12° (from Me2CO-Et2O). IV (2.5 g.) in 100 cc. H2O adjusted to pH 7.0-7.5 with 2N LiOH, treated with 1 g. renal acylase I, diluted to 130 cc., incubated about 4 hrs. at 39°, concentrated to 50 cc. in vacuo, dialyzed 4 times against 750 cc. H2O, the combined dialyzates (3 l.) concentrated to 15 cc. in vacuo, adjusted to pH 3.4 with 6N HCl, concentrated to beginning crystallization, diluted with 50 cc. absolute EtOH, and kept 24 hrs. at room temperature gave 800 mg. L-III, [α]D26 21.5° (c 1, 5N HCl); the filtrate acidified to pH 1.7, evaporated to dryness in vacuo, and extracted with boiling Me2CO, the extract concentrated in an air stream, the residual oil refluxed 2 hrs. with 125 cc. 2N HCl and evaporated to dryness in vacuo, the residue dissolved in a little H2O, the pH adjusted to 3.4 with 2N LiOH, and the solution concentrated to beginning crystallization and diluted with absolute EtOH yielded 500 mg. D-III, [α]D26 -21.0° (c 1, 5N HCl). D- and L-III gave the following Rf values (developer, and paper given): 0.44, PhOHNH4OH, Whatman Number 4; 0.43, 4:1:5 BuOH-AcOH-H2O, Whatman Number 4; 0.73, 10:77:20 pyridine-MeOH-H2O, Whatman Number 1. A mixture of the 3 isomers of CH2[CH2CH(NH2)CO2H]2 (V) was prepared in essentially the same manner in 66% yield; it showed 2 ninhydrin-sensitive spots with Rf values 0.46 and 0.57 corresponding to meso-V and D- and L-V. V (9.5 g.) in 125 cc. 2N NaOH treated with 19.5 cc. PhCH2OCOCl in portions with cooling and stirring during about 0.5 hr., the mixture shaken 2 hrs. at room temperature and washed with EtOAc, the aqueous layer acidified to pH 1.7 with 4N

HCl, the precipitated oil extracted into EtOAc, the extract dried, concentrated to 50°
in vacuo, kept at 4° overnight, and filtered, and the filter residue recrystd. from EtOAc gave 6.0 g. di(carbobenzyloxy) derivative (VI) of DL-V, m. 164-5° with shrinking at 155°. The combined EtOAc mother liquors from VI evaporated, and the gummy residue crystallized from hot CHCl3 gave 6.2 g. meso-isomer (VII) of VI, m 123-5°. VII (30 g.) in 300 cc. AcOH and 100 cc. H2O hydrogenated over Pd black, filtered, concentrated in vacuo, diluted with 50 cc., evaporated again, and recrystd. twice from
35% aqueous EtOH yielded 7.5 g. meso-V, Rf 0.45. VI (45.8 g.) and 27.8 cc. Et3N in 600 cc. dioxane treated slowly with cooling with 24.4 cc. iso-BuCOCl below 12°, kept 1 hr. at 10°, treated dropwise with 26 cc. NH4OH(d. 0.90), allowed to stand 16 hrs., and filtered by suction yielded 18.0 g. diamide (VIII) of VI, mass of needles, m. 223-4° (from aqueous HCONMe2). VIII (21.5 g.) hydrogenolyzed in 400 cc. AcOH over Pd black, filtered, evaporated, diluted with 25 cc. H2O, and again
evaporated, the residual oil dissolved in 300 cc. H2O containing 1.15 g. Mn(OAc)2.4H2O, the pH adjusted to 6.5 with 2N LiOH, the mixture treated with 1.8 g. lyophilized amidase powder, the pH adjusted to 8.0 with 2N LiOH, diluted to 470 cc., kept 5 hrs. at 38°, concentrated to about 50 cc., dialyzed 4 times against H2O (about 900 cc. each time) at 5°, the combined dialyzates concentrated to about 50 cc. in vacuo, passed through Amberlite XE-64 (Li+ form), and collected in 20-cc. fractions, the combined fractions 19-31 evaporated to dryness, the residue dissolved in the min. amount of hot H2O, the solution treated with C, filtered, adjusted to pH 6.5 with 2N LiOH, and diluted with 4 vols. absolute EtOH, and the white amorphous precipitate reppted. twice in the same manner yielded 3.5 g. L-V, Rf 0.57, [α]D26 45.0° (c 1, N HCl). The fractions from number 176 on combined and evaporated in vacuo, the residual sirup refluxed 6 hrs. with 1 l. 3N HCl, evaporated, dissolved in 1.5N HCl, and passed through Dowex 50, and the effluent adjusted to 2.5N HCl and evaporated gave 2.9 g. D-V, [α]D26-45.5° (c 1, N HCl). The infrared absorption spectra of L-III, meso-V, and DL-V are recorded.

IT 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 109815-40-9 CAPLUS

CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)



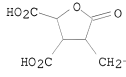
● K

L10 ANSWER 42 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1951:41362 CAPLUS
DOCUMENT NUMBER: 45:41362
ORIGINAL REFERENCE NO.: 45:7056c-i,7057a-d
TITLE: Natural tannins. V. Constitution of the "fission acid," C14H12O11, obtained from chebulinic and chebulagic acid
AUTHOR(S): Schmidt, Otto Th.; Mayer, Walter
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Annalen der Chemie, Justus Liebigs (1951), 571, 1-15
CODEN: 9X224Y
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 45, 1544d. The tri-Me derivative (I) of the "fission acid" ("Spaltsaure") (II) (cf. C.A. 44, 9176a) when neutralized and treated in aqueous EtOH with p-BrC6H4COCH2Br gave a tris(p-bromophenacyl)ester, C41H33O14Br3, micro droplets, glassy (purified by repeated solution in hot alc. and precipitation with H2O). The tris-(p-phenylphenacyl) ester, C39H48O14, forms glassy droplets. The hexa-Me derivative (III) of II on standing 2 days with MeOH-NH3 (saturated at -10°), followed by refluxing with PrOH and cooling to 0° gave trimethyl fission acid triamide, [C17H21O8N3 (IV), macroprisms, m. 257° (decomposition) (from EtOH or H2O), [α]20D 48.7 ± 3° (H2O, 20 min. after solution, c 1.9). III, b0.01 202-4°, [α]20D 49.3° (± 0.8°) (MeOH, c 2.3) prepared from I in Me2CO by treatment with CH2N2 in Et2O. Zerewitinoff detns. of "active H" in III gave very low fluctuating results [corresponding to about 0.3 mole H, indicating that the Grignard reagent reacted very sluggishly with H attached to a C atom (cf. Meunier, Bulletin society chim. (3) 29, 1177(1903)], and that no free HO groups are present in III. When I was titrated with 0.1 N NaOH (either directly or by using an excess of the reagent) 3 equivs. of alkali were used in the neutralization. However, when I was heated at 100° with an excess of 2 N NaOH, the back-titration with acid indicated the presence of a 4th CO2H group and an amorphous tetra-Na salt, C17H16O12N4 (V), was recovered by precipitation from the alkaline solution with MeOH. This behavior indicates an aromatic lactone in II. With HCl, V is reconverted into I. To 4 g. I in 60 cc. ice-cold H2O was added 40 cc. H2O, the cooled, stirred mixture treated dropwise (at temps. not above 0°) with 220 cc. N KMnO4 in the course of 10 hrs., then with another 60 cc. H2SO4, allowed to stand overnight, extracted 4 days with Et2O in a Schacherl apparatus, and the extract concentrated, treated with 25 cc. H2O, reextd. with Et2O and treated with CH2N2, giving 0.75 g. OC.CH(CH2CO2Me).CH(CO2Me).CH(CO2Me).O (VI), b0.02 150-3°, m. 81-2° (from Me2CO-H2O or C6H6-cyclohexane), [α]20D 117.5° (± 0.9°) (c 2.2, MeOH). When saponified 2 hrs. with N NaOH (or 4 hrs. with 0.1 N NaOH), followed by back titration, VI consumed 4 equivs. of alkali; the tetra-Na salt, C8H6O9N4 (VII), a neutral microcryst. hygroscopic powder precipitated from the alkaline solution with MeOH, [α]20D -4.9 ± 1° (H2O, c 1), gave rise to white, flocculent, insol. Pb, Ba, and Ag salts (but yielded no ppts. with CaCl2 or CuSO4). VII (0.9 g.) in an excess of N HCl, extracted with Et2O, gave 0.55 g. OC.CH(CH2CO2H)CH(CO2H).CH(CO2H).O (VIII), m. 200-7° (decomposition) (from Et2O), [α]20D 104.9° (± 0.7°) (c 3, H2O in 15 min.), 85.9° (after 16 days). VIII heated 1 hr. with concentrated H2SO4 or 3 hrs. with 50% H2SO4 remained unchanged. Heating VIII with PhNHMe at 186° gave no CO2. Whereas VII gave a blue color with K2Cr2O7 and HNO3, VIII gave no such coloration (cf. Fearon and Mitchell, C.A. 26, 4011). VI (0.438 g.) and MeOH-NH3 gave (after several

days at room temperature and 1 day at 0°) 0.1 g. of a tetraamide, C18H14O5N4, hexagons, m. 211° (decomposition) (from 45% EtOH), and from the mother liquors after refluxing 1 hr., 0.1 g. of the triamide lactone, C8H11O5N3 (corresponding to VIII), needles, m. 216° (decomposition) (from 80% EtOH). VI (1.01 g.) in 5 g. KOH and 5 cc. H2O was heated successively 0.5 hr. each at 100°, 180°, and 210-20°, and the cooled mixture acidified with 4 N H2SO4 and extracted with Et2O in a Schacherl apparatus, giving a mixture of 0.095 g. AcOH, and (after methylation) 0.3 g. (CO2Me)2, m. 53°, and 0.35 g. (CH2CO2Me)2 [identified as (CH2CONH2)2, m. 258°]. Isocitric acid lactone (IX), m. 162-3° (1.7 g.), treated similarly with KOH gave 1.74 mole AcOH and 0.73 mole (CO2H)2. Tricarballylic acid, m. 164°, similarly treated, was recovered unchanged. MeCH(OH)CH2CO2H on alkaline fusion yielded nearly 2 moles AcOH. These data indicate that VI cannot have the structure OC.O.CH(CO2H).C(CH2CO2H)(CO2H)CH2. O.CO.CH2.CH(CO2Me).C(CO2Me)CH2CO2Me (0.2 g.), the synthesis of which is reserved for future publication, when saponified with 5 cc. N NaOH and oxidized with 20 cc. N KMnO4 and 15 cc. N NaOH gave approx. 0.32 mole (CO2H)2 [isolated as (CO2)2Ca]. Under similar conditions 0.2 g. VI gave 2.58 moles (i.e. 65% of 4 moles) (CO2H)2. IX gave 2.32 moles, citric acid 0.24 mole, malic acid 1.7 moles, and HO2CCOCH2CO2H 1.8 moles (CO2H)2. Subjected to similar treatment, pure (CO2Na)2 remained unchanged. A mixture of 1.186 g. IV, 20 cc. and hypochlorite solution containing 0.88 g. NaOCl and
10
cc. 2 N NaOH was shaken 0.5 hr. and heated 15 min. on a steam bath; the excess NaOCl destroyed by solid Na2S2O3, and the mixture neutralized with AcOH and treated with NH2NHCONH2.HCl and AcONa, yielding 0.298 g. (H2NCONH)2, m. 258° (derived from NaNCO), thus indicating that the HO group involved in lactone formation in II is on an α-C atom. From various data, a structure for II is proposed.

IT 1129294-31-0P
RL: SPN (Synthetic preparation); PRP (Properties); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(Natural tannins. V. Constitution of the "fission acid," C14H12O11, obtained from chebulinic and chebulagic acid)

RN 1129294-31-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

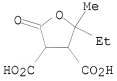


L10 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1927:23508 CAPLUS
DOCUMENT NUMBER: 21:23508
ORIGINAL REFERENCE NO.: 21:2877h-i
TITLE: Influence of groups and associated rings on the stability of certain heterocyclic systems. III. The substituted pareconic acida
AUTHOR(S): Sircar, S. S. G.
SOURCE: Journal of the Chemical Society (1927) 1257-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

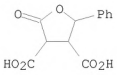
AB The following values of k + 105 were observed for paraconic acid and its derivs.: acid., 1630; Me derivative, 763; Et derivative, 652; di-Me derivative, 270; MeEt derivative, 164; di-Et derivative, 74.5°; cyclopentane derivative, 119; cyclohexane derivative, 107. 2,3.Dicyano-1-methyl-1-ethylcyclopropane-2-carboxylamide, m. 127-8° (from the imide, m. 225-7°); the γ-lactone of β-hydroxy-β-ethylbutane-γ,δ,δ,-tricarboxylic acid, m. 157-8° (decomposition); methylethylparaconic acid, m. 131-2° (Ag salt). Cyclopentanespiro-2,3-dicyanocyclopropane-2-carboxylamide, m. 126° (from the imide, m. 202-3°); the γ-lactone of 1-hydroxycyclopentylethane-α,β,β tricarboxylic acid, m. 175-7° (decomposition); heating at 200° for 2 hrs. gives cyclopentanespiroparaconic acid, m. 127° (Ag salt).

IT 857821-26-2P, 1,1,2-Pentanetricarboxylic acid, 3-hydroxy-3-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

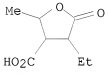
RN 857821-26-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



L10 ANSWER 44 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1925:20338 CAPLUS
DOCUMENT NUMBER: 19:20338
ORIGINAL REFERENCE NO.: 19:2643d-i,2644a
TITLE: Conditions underlying the formation of unsaturated and cyclic compounds from halogenated open-chain derivatives. VII. The influence of the phenyl group on the formation of the cyclopropene ring
AUTHOR(S): Haerdi, Wilhelm; Thorpe, J. F.
SOURCE: Journal of the Chemical Society, Transactions (1925), 127, 1237-48
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB An attempt was made to prepare the acid I which, in its semi-aromatic form, would have the structure II, in order to supply further evidence in support of reported views regarding the structure of the semi-aromatic ring type of which the acid III is at present the only known member. I was not obtained but the effect of the Ph group on 3-C ring formation was studied. PhCH(CH2CO2H)2, PCl5 and Br, warmed for 2 hrs. and then poured into MeOH gave Me α-bromo-β-phenylglutarate (IV), b17 204-6°, m. 86-7°; larger amts. of Br gave the α,α'-di-Br derivative, b20 215-20°, m. 82.5-3.5°, whose Et ester (V) is a viscous liquid. The free acid m. 192-3°. Distillation of V in vacuo gives the lactone of Et α-bromo-α'-hydroxy-β-phenylglutarate, (VI), b21 230-4°. Hydrolysis of IV gave PhCH(CH2CO2H)2, when MeOH-KOH was used, or the Me ester when C5H5N was used. V (or the Me ester) and MeOH-KOH did not give the expected I but a mixture of 10% PhCH: CHCO2H and (CO2H)2 and 2-ethoxy-3-phenylcyclopropane-1,2-dicarboxylic acid, m. 198-9°, stable towards alkaline KMnO4 for 24 hrs. Me ester, b13 175-9°; Et ester, b14 184-90°. VI gave the same products but the PhCH:CHCO2H and (CO2H)2 were present in larger amts. Me 1-bromo-3-phenylcyclopropane-1,2-dicarboxylate (VII), oil which solidifies in a freezing mixture; the Br acid ester m. 175-6°. The bromination proceeds in the absence of a catalyst but in the light of an arc-lamp at 125-40°. Dibromination gave a product, C11H9O4Br(?), m. 227-8°, which may be a Br-acid or a bromolactonic acid. Hydrolysis of these esters gives phenylcyclopropanedicarboxylic acid, m. 175-6°. Et α-carbethoxy-α'-bromo-β-phenylglutaconate, on hydrolysis with aqueous KOH, gives 60-70% BzCH2CH(CO2H)2; in EtOH the hydrolysis gives BzCH2CH2CO2Et; after standing 2 days with EtOH-NH3 a compound containing both N and Br seps. PhCHBrCHBrCO2Et and CHNa(CO2Et)2 gave as the main product Et phenylcyclopropanetricarboxylate, b16 108-11°. Hydrolysis of the ester gave carboxyphenylparaconic acid (VIII), prisms with 4 H2O, m. 88°, or anhydrous, m. 187-8°; boiling with HCl gives phenylparaconic acid, m. 99-100°. PhCBr:CBrCO2Et and CHNa(CO2Et)2, condensed with 1 mol. EtONa, give an acid, C14H12O6, m. 171-2°, probably containing a lactone ring. Boiling with HCl gives phenylparaconic acid. In the absence of EtOH there results the ester EtO2CCH: CPhCBr(CO2Et)2, b16 201-5°; it reduces KMnO4 but does not react with Br in CHCl3. The ester is unchanged by the action of Na in C6H6 or PhMe; hydrolysis with 60% KOH gives VIII.
IT 861321-23-5P, 3,4-Furandicarboxylic acid, tetrahydro-2-keto-5-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 861321-23-5 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-phenyl- (CA INDEX NAME)


O
O
Ph
HO2C
CO2H

L10 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1910:4532 CAPLUS
DOCUMENT NUMBER: 4:4532
ORIGINAL REFERENCE NO.: 4:771c-f
TITLE: α-Ethylpentenoic Acid and Xeronic Anhydride
AUTHOR(S): Fichter, Fr.; Obladen, Hans
CORPORATE SOURCE: I. Univ. Lab., Basel
SOURCE: Berichte der Deutschen Chemischen Gesellschaft (1910), 42, 4703-7
CODEN: BDCGAS; ISSN: 0365-9496
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Et α-ethylacetsuccinate, EtO2CCHAcCHEtCO2Et, when reduced with Na-Hg, gives α-ethyl-γ-methylparaconic acid, formula (I) below; small needles from petroleum ether, m. 111°, b12 192-6°. When carefully and slowly distilled, under the ordinary pressure, it gives a mixture of α-ethyl-β,γ-pentenoic acid and xeronic anhydride, which are separated by means of their Ba salts, the former being the more readily soluble α-Ethyl-β,γ-pentenoic acid, MeCH : CHCHEtCO2H; oil, b12 116°; K 0.00339, at 25°. Prolonged boiling with aqueous NaOH (20%) in excess converts it into α-ethyl-α,β-pentenoic acid, EtCH : CEtCO2H; b12 120°; m. below 0°; K 0.00205, at 25°. Barium salt, small needles with 1 H2O. Prolonged boiling of xeronic anhydride (II), with aqueous NaOH transforms it into α-ethyl-γ-methylitaconic acid, MeCH: C(CO2H)CHEtCO2H; slender crystals from H2O, m. 136°. Anhydride, formed by the action of AcCl; colorless oil, b12 142-4°. p-Tolil, bundles of small needles from petroleum ether, m. 84°; b12 220°. Xeranic p-tolil, needles from petroleum ether, m. 107° (cf. following abstract).
IT 861071-03-6P, Paraconic acid, 4-ethyl-2-methyl-
RL: PREP (Preparation)
(preparation of)
RN 861071-03-6 CAPLUS
CN 3-Furancarboxylic acid, 4-ethyltetrahydro-2-methyl-5-oxo- (CA INDEX NAME)



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FULL ESTIMATED COST                                    254.05     814.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -36.08     -36.08

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     FILE 'REGISTRY' ENTERED AT 18:48:46 ON 20 JUL 2009
L1             STRUCTURE UPLOADED
L2          604 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 18:49:11 ON 20 JUL 2009
L3          757 S L2 FULL

     FILE 'REGISTRY' ENTERED AT 18:50:09 ON 20 JUL 2009
L4             STRUCTURE UPLOADED
L5          183 S L4 FULL

     FILE 'CAPLUS' ENTERED AT 18:50:44 ON 20 JUL 2009
L6          142 S L5 FULL

     FILE 'REGISTRY' ENTERED AT 18:52:27 ON 20 JUL 2009
L7             STRUCTURE UPLOADED
L8          100 S L7 FULL

     FILE 'CAPLUS' ENTERED AT 18:52:57 ON 20 JUL 2009
L9           97 S L8 FULL
L10          45 S L6 NOT L9

     FILE 'STNGUIDE' ENTERED AT 18:55:38 ON 20 JUL 2009

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=> FILE REG
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                      1.19     815.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                      0.00     -36.08

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DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

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6 7 8 9 12 13 14 15
ring nodes :
1 2 3 4 5
chain bonds :

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1-7  2-12  2-14  4-6  5-13  5-15  7-8  7-9
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
2-12  4-6  5-13
exact bonds :
1-2  1-5  1-7  2-3  2-14  3-4  4-5  5-15
normalized bonds :
7-8  7-9
isolated ring systems :
containing 1 :


G1:Cy,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS
12:CLASS  13:CLASS  14:CLASS  15:CLASS



L11     STRUCTURE UPLOADED

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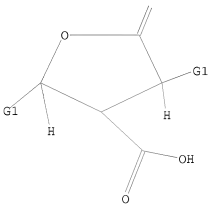


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G1 Cy,Ak


Structure attributes must be viewed using STN Express query preparation.


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FULL SCREEN SEARCH COMPLETED -     1817 TO ITERATE

100.0% PROCESSED     1817 ITERATIONS                              150 ANSWERS
SEARCH TIME: 00.00.01

L12         150 SEA SSS FUL L11

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COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
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FULL ESTIMATED COST                                  185.88    1001.48
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CA SUBSCRIBER PRICE 0.00 -36.08

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FILE COVERS 1907 - 20 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 19 Jul 2009 (20090719/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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information. This enhancement may impact record import into
database management software. For additional information, refer
to NEWS 22.

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L13         125 L12

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            125 L12
L14          94 L12 NOT L10

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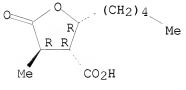
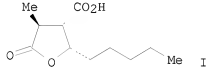
L14 ANSWER 1 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:994706 CAPLUS
DOCUMENT NUMBER: 149:307103
TITLE: Indium
AUTHOR(S): Lowinger, Timothy B.; Loh, Teck Peng
CORPORATE SOURCE: USA
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis (2001), No pp. given. John Wiley & Sons, Ltd.: Chichester, UK.
CODEN: 69KUHI
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME
DOCUMENT TYPE: Conference; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:307103
AB A review of the article Indium.
IT 203514-35-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Indium)
RN 203514-35-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



L14 ANSWER 2 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:580890 CAPLUS
DOCUMENT NUMBER: 149:128665
TITLE: Concise syntheses of (+)- and (-)-methylenolactocins and phaseolinic acids
AUTHOR(S): Hajra, Saumen; Karmakar, Ananta; Giri, Aswini Kumar; Hazra, Sunit
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kharagpur, 721 302, India
SOURCE: Tetrahedron Letters (2008), 49(22), 3625-3627
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:128665
GI



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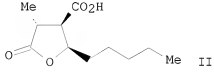
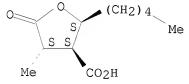


II

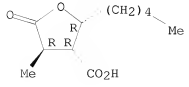
AB (+)- And (-)-Methylenolactocins and phaseolinic acids, e.g. I and II, are synthesized in four steps via asym. syn- and anti-aldol reactions of chiral N-succinyl-2-oxazolidinones using the same set of reagents.
IT 109667-12-1P 185246-65-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. syntheses of (+)- and (-)-methylenolactocins and phaseolinic acids)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 185246-65-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)- (CA INDEX NAME)

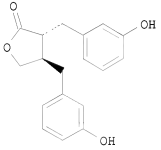
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1170881 CAPLUS
DOCUMENT NUMBER: 148:54779
TITLE: Convenient route to enantiopure substituted butyrolactones: application in a formal synthesis of both enantiomers of enterolactone
AUTHOR(S): Ghosh, Manju
CORPORATE SOURCE: Department of Organic Chemistry, Indian Association for the Cultivation of Science, Kolkata, 700032, India
SOURCE: Tetrahedron (2007), 63(47), 11710-11715
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:54779
GI



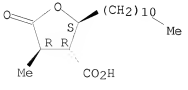
I

AB A simple route for the synthesis of enantiopure substituted γ-butyrolactones involving a highly diastereoselective alkylation of an enantiomerically pure substituted latent succinate ester was described. This route provides entry into both enantiomers of 3,4-disubstituted butyrolactones from a single enantiomer of a (+)-(R)-2,3-cyclohexylideneglyceraldehyde derivative The synthetic potential of this methodol. was demonstrated by a formal synthesis of both (3R,4R)-enterolactone (I) and its (3S,4S)-enantiomer.

IT 480-71-7DP, Nephrosteranic acid, analogs 19464-85-8DP, Roccellaric acid, analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(formal synthesis of both enantiomers of enterolactone via diastereoselective alkylation)

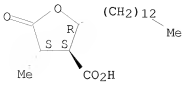
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



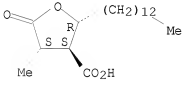
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:840348 CAPLUS
DOCUMENT NUMBER: 147:371328
TITLE: Separation of a mixture of paraconic acids from Cetraria islandica (L.) Ach. employing a fluorous tag-catch and release strategy
AUTHOR(S): Horhant, David; Le Lamer, Anne-Cecile; Boustie, Joeel; Uriac, Philippe; Gouault, Nicolas
CORPORATE SOURCE: UFR Sciences Pharmaceutiques et Biologiques, Universite de Rennes 1, Rennes, 35043, Fr.
SOURCE: Tetrahedron Letters (2007), 48(34), 6031-6033
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:371328

AB A light-fluorous catch and release approach application has been designed to the separation of a mixture of three paraconic acids extracted from the Island moss (Cetraria islandica (L.) Ach.). The (+)-protolichesterinic acid was caught and released via a Michael/retro-Michael addition sequence with a fluorous thiol, while the resulting two other compds. were classically separated, allowing the isolation of (+)-roccellaric acid for the first time in this lichen.

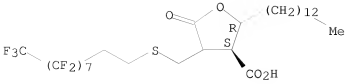
IT 19464-85-8P, (+)-Roccellaric acid
RL: BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(separation of a mixture of paraconic acids from Cetraria islandica employing a fluorous tag-catch and release strategy)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



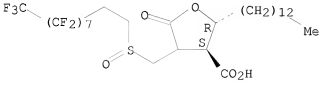
IT 949535-89-1P 949535-90-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(separation of a mixture of paraconic acids from Cetraria islandica employing a fluorous tag-catch and release strategy)
RN 949535-89-1 CAPLUS
CN 3-Furancarboxylic acid, 4-[[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]methyl]tetrahydro-5-oxo-2-tridecyl-, (2R,3S)- (CA INDEX NAME)

Absolute stereochemistry.



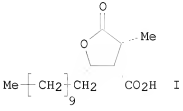
RN 949535-90-4 CAPLUS
CN 3-Furancarboxylic acid, 4-[[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)sulfinyl]methyl]tetrahydro-5-oxo-2-tridecyl-, (2R,3S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:554240 CAPLUS
DOCUMENT NUMBER: 147:188978
TITLE: Dibromomethane as One-Carbon Source in Organic Synthesis: Formal Total Synthesis of (±)-Nephrosteranic Acid
AUTHOR(S): Hon, Yung-Son; Hsieh, Cheng-Han; Chen, Hsien-Fan
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Institute of Chemistry, Academia Sinica, National Chung Cheng University, Chia-Yi, Taiwan
SOURCE: Synthetic Communications (2007), 37(10), 1635-1651
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:188978
GI

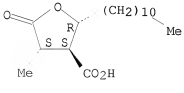


AB A diastereoselective formal total synthesis of (±)-nephrosteranic acid (10) is described. The key step is to introduce the α-methylene group by the ozonolysis of monosubstituted alkenes followed by reaction with a preheated mixture of CH2Br2-Et2NH. The α-Me group of compound I was formed from the reduction of the corresponding α-methylene precursor.

IT 922524-70-7P, (±)-Nephrosteranic acid 944339-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(formal total synthesis of (±)-nephrosteranic acid with the ozonolysis of monosubstituted alkenes followed by reaction with a preheated mixture of CH2Br2-Et2NH as key step)

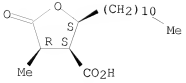
RN 922524-70-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 944339-95-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

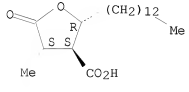
L14 ANSWER 6 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:503001 CAPLUS
DOCUMENT NUMBER: 148:449352
TITLE: General enantioselective synthesis of butyrolactone natural products via ruthenium-SYNPHOS-catalyzed hydrogenation reactions
AUTHOR(S): Blanc, Delphine; Madec, Jonathan; Popowyck, Florence; Ayad, Tahar; Phansavath, Phannarath; Ratovelomanana-Vidal, Virginie; Genet, Jean-Pierre
CORPORATE SOURCE: Laboratoire de Synthese Selective Organique et Produits Naturels, Ecole Nationale Superieure de Chimie de Paris, UMR 7573 CNRS, Paris, 75231/05, Fr.
SOURCE: Advanced Synthesis & Catalysis (2007), 349(6), 943-950
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Enantioselective syntheses of several paraconic acids were achieved using catalyzed asym. hydrogenation of β-keto esters with SYNPHOS as a ligand. This strategy allowed the short synthesis of biol. active (-)-methylenolactocin, (-)-protolichesterinic acid, (-)-phaseolinic acid, and (+)-roccellaric acid.

IT 19464-85-8P, (+)-Roccellaric acid 109667-12-1P, (-)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective synthesis of butyrolactone natural products via ruthenium-SYNPHOS-catalyzed hydrogenation)

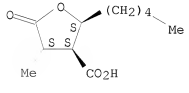
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



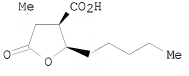
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

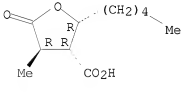
L14 ANSWER 7 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:187851 CAPLUS
DOCUMENT NUMBER: 146:421762
TITLE: Synthesis of substituted butenolides by the ring closing metathesis of two electron deficient olefins: a general route to the natural products of paraconic acids class
AUTHOR(S): Selvakumar, N.; Kumar, P. Kalyan; Reddy, K. Chandra Shekar; Chary, B. Chandra
CORPORATE SOURCE: Department of Discovery Chemistry, Discovery Research, Dr. Reddy's Laboratories Ltd., Miyapur, Hyderabad, 500 049, India
SOURCE: Tetrahedron Letters (2007), 48(11), 2021-2024
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:421762
GI



I

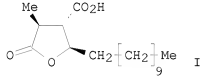
AB A variety of allyl acrylates possessing electron-withdrawing groups undergo RCM using the second generation Grubbs' catalyst in the presence of a Lewis acid resulting in diverse butenolides in high isolated yields. This methodol. provides a general route to the natural products of paraconic acids class, exemplified by a total synthesis of (±)-phaseolinic acid (I).
IT 203514-35-6P, (±)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of substituted butenolides by ring closing metathesis of two electron deficient olefins with application synthesis of paraconic acid, (±)-phaseolinic acid)
RN 203514-35-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

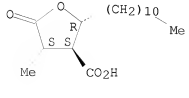
L14 ANSWER 8 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1287478 CAPLUS
DOCUMENT NUMBER: 146:206134
TITLE: α,β-Unsaturated diesters: radical acceptors in dialkylzinc-mediated tandem radical addition/aldol condensation. A straightforward synthesis of (±)-nephrosteranic acid
AUTHOR(S): Bazin, Samantha; Feray, Laurence; Vanthuyne, Nicolas; Siri, Didier; Bertrand, Michele P.
CORPORATE SOURCE: Laboratoire de Chimie Moleculaire Organique, UMR 6517, Faculte des Sciences St. Jerome, Universite Paul Cezanne, Marseille, 13397, Fr.
SOURCE: Tetrahedron (2006), Volume Date 2007, 63(1), 77-85
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:206134
GI



I

AB The sequence involving conjugate radical addition/aldol condensation/lactonization is a high yielding route to di- and tri-substituted γ-lactones starting from fumaric or maleic diesters. The reactions are mediated with dialkylzincs. The domino process relies on the ability of dialkylzinc to transform α-alkoxycarbonylalkyl radicals into zinc enolates. Compared to diethylzinc, dimethylzinc enables the use of a wider range of alkyl radical precursors. In addition, dimethylzinc is a convenient source of Me radical, which leads to a straightforward synthesis of methylated derivs. related to α-methyl-paraconic acids, and specifically the title acid I.
IT 922524-70-7P, (±)-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of (±)-nephrosteranic acid via dialkylzinc-mediated tandem radical addition/aldol condensation of α,β-unsatd. diesters)
RN 922524-70-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



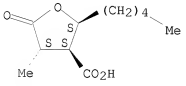
REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 9 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1140725 CAPLUS
DOCUMENT NUMBER: 146:100326
TITLE: Catalytic Asymmetric Synthesis of Acyclic Arrays by Tandem 1,4-Addition-Aldol Reactions
AUTHOR(S): Howell, Gareth P.; Fletcher, Stephen P.; Geurts, Koen; ter Horst, Bjorn; Feringa, Ben L.
CORPORATE SOURCE: Department of Organic Molecular Inorganic Chemistry, Stratingh Institute, University of Groningen, Groningen, 9747 AG, Neth.
SOURCE: Journal of the American Chemical Society (2006), 128(46), 14977-14985
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:100326

AB Herein, the efficient acyclic stereocontrol in tandem 1,4-addition-aldol reactions triggered by catalytic asym. organometallic addition is reported. Grignard reagents, e.g. methylmagnesium bromide, add to α,β-unsatd. thioesters R1CH:CHC(O)SMe (R1 = Ph, 4-C1C6H4, Me3CSiPh2OCH2) in a 1,4-fashion and the resulting magnesium enolates are trapped with aromatic or aliphatic aldehydes R2CHO (R2 = Me3C, n-pentyl, cyclohexyl, Ph, 4-BrC6H4, 4-O2NC6H4, 4-MeOC6H4). The process provides a range of tandem products R1CHMeCH(CO2Me)CHR2OH bearing three contiguous stereocenters with excellent control of relative and absolute stereochem. The various diastereomeric products have been fully characterized using single-crystal X-ray anal. and the origins of stereocontrol in this tandem protocol are discussed. The versatility and efficiency of this methodol. are demonstrated in the first catalytic asym. synthesis of (-)-phaseolinic acid with 54% overall yield via a short and concise route.

IT 109667-12-1P, (-)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of (-)-phaseolinic acid from α,β-unsatd. thioester via Cu/JOSIPHOS-catalyzed tandem conjugate Grignard addition-aldol condensation)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



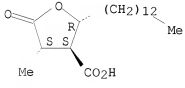
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:477335 CAPLUS
DOCUMENT NUMBER: 145:124363
TITLE: Enantioselective butenolide preparation for straightforward asymmetric syntheses of γ-lactones - paraconic acids, avenaciolide, and hydroxylated eleutherol
AUTHOR(S): Braukmueller, Stefan; Brueckner, Reinhard
CORPORATE SOURCE: Institut fuer Organische Chemie und Biochemie, Albert-Ludwigs-Universitaet, Freiburg, 79104, Germany
SOURCE: European Journal of Organic Chemistry (2006), (9), 2110-2118
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124363
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB ZThe naturally occurring γ-lactones (+)-methylenolactocin (I) and its enantiomer, (+)-protolichesterinic acid (II) and its enantiomer, (+)-rocellaric acid (III), and the methylene bis(γ-lactone) (-)-avenaciolide (IV) were synthesized with 95-98% ees in very few steps. Enantiocontrol was imposed by the asym. dihydroxylation of trans-configured β,γ-unsatd. carboxylic esters. β,γ-Unsatd. carboxylic ester V required increased amts. of the oxidant and auxiliary to produce the hydroxy lactone, a precursor of the naphtho-γ-lactone (+)-9-hydroxyeleutherol (VI).
IT 19464-85-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective butenolide preparation for straightforward asym. syntheses of γ-lactones, paraconic acids, avenaciolide, and hydroxylated eleutherol)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



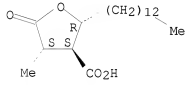
REFERENCE COUNT: 117 THERE ARE 117 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 11 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:213181 CAPLUS
DOCUMENT NUMBER: 145:140805
TITLE: Two aliphatic acid derivatives from the cultured mycobionts of Lecanora nipponica
AUTHOR(S): Takenaka, Yukiko; Hamada, Nobuo; Tanahashi, Takao
CORPORATE SOURCE: Kobe Pharmaceutical University, 4-19-1, Motoyamakita-machi, Higashinada-ku, Kobe, 658-8558, Japan
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2005), 60(12), 1324-1326
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Spore-derived mycobionts of the lichen Lecanora nipponica were cultivated on a malt-yeast extract medium supplemented with 10% sucrose and their metabolites were investigated. Two new metabolites, Me (2Z,4E)-3-methoxycarbonyl-2-methyl-2,4-nonadienoate and (4E)-3-methoxycarbonyl-2-methyl-4-nonenoic acid, were isolated. Their structures were determined by spectroscopic methods.

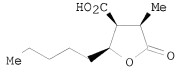
IT 19464-85-8
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure of)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

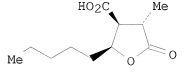


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:153612 CAPLUS
DOCUMENT NUMBER: 144:369810
TITLE: A versatile stereoselective approach to paraconic acids
AUTHOR(S): Amador, Marta; Ariza, Xavier; Garcia, Jordi
CORPORATE SOURCE: Department of Organic Chemistry, University of Barcelona, Barcelona, 08028, Spain
SOURCE: Heterocycles (2006), 67(2), 705-720
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369810
GI



I



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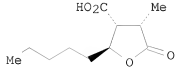
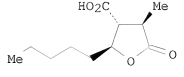


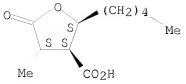
III



IV

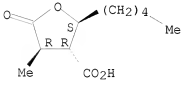
AB A versatile methodol. was developed for the independent stereochem. control in the construction of all the stereocenters of the γ-butyrolactone skeleton that are present in paraconic acids. The configuration of the γ-carbon came from an enantiopure alk-2-yne-1,4-diol. Stereoselective partial reduction to a O-acylated (Z)- or (E)-alkenediol controlled the stereochem. of the β-carbon whereas the α-carbon stereochem. in 1 was partially selected by a (Z)- or (E)-enolate formation of the 1,4-dipropanoate derived from the alk-2-ene-diol. E.g., (S,S,Z)-Me(CH2)4CH(OCOCH2Me)CH:CHCH(OCOCH2Me)(CH2)4Me was converted by this methodol. to cis,cis- and trans,cis-γ-butyrolactone acids I and II. Similarly, the corresponding O-acylated (S,S,E)-alkenediol lead to cis,trans- and trans,trans-γ-butyrolactone acids III and IV.
IT 109667-12-1P 203864-73-7P 807346-05-0P
882161-96-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthetic route to paraconic acids)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



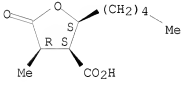
RN 203864-73-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3R,4R)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



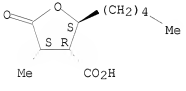
RN 807346-05-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4R)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 882161-96-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3R,4S)-
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

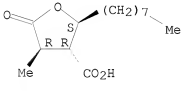
L14 ANSWER 13 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:708473 CAPLUS
DOCUMENT NUMBER: 143:326143
TITLE: New α-methylene-γ-butyrolactones with antimycobacterial properties
AUTHOR(S): Hughes, Minerva A.; McFadden, Jill M.; Townsend, Craig A.
CORPORATE SOURCE: Department of Chemistry, The Johns Hopkins University, Baltimore, MD, 21218, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(17), 3857-3859
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:326143

AB The synthesis and antimycobacterial activity of a series of α-methylene-γ-butyrolactones based on the natural product protolichesterinic acid are described. The products bearing an allylamide group at the C-4 position showed improved activity with MICs in the range of 6.25-12.5 μg/mL.

IT 647830-52-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of α-methylene-γ-butyrolactone derivs. and study of their antimycobacterial activity)

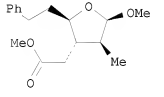
RN 647830-52-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 14 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:277465 CAPLUS
DOCUMENT NUMBER: 142:481867
TITLE: Facially controlled C-methylation of oxolanyl and cyclopentyl acetate enolates: application to the total synthesis of (+)-nephromopsinic acid
AUTHOR(S): Mulzer, Johann; Steffen, Ulrich; Martin, Harry J.; Zorn, Ludwig
CORPORATE SOURCE: Institut fuer Organische Chemie der Universitaet Wien, Vienna, 1090, Austria
SOURCE: European Journal of Organic Chemistry (2005), (6), 1028-1043
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:481867
GI



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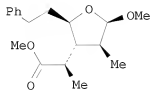
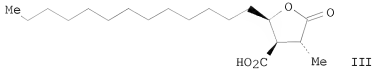


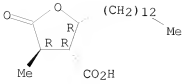
II



III

AB The stereoselectivity of the C-methylation of oxolanyl and cyclopentyl acetate enolates, e.g. I, was investigated. The configuration of the C-Me diastereomers, e.g. II, was elucidated by a combination of crystal structure anal., NMR spectroscopy and chemical correlations. Generally, the methylation proceeded re*-selectively, although with very different degrees of selectivity. The most important stereodirecting effect was a steric one exerted by the 5-phenethyl substituent, and this steric effect was strongly increased by the stereodirecting effect of a 3-OR group. Contrary to previous literature evidence, the endocyclic oxolanyl oxygen does not exert an effect. These findings were applied in a highly stereoselective synthesis of (+)-nephromopsinic acid (III).
IT 133695-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(facially controlled C-methylation of oxolanyl and cyclopentyl acetate enolates and application to the total synthesis of (+)-nephromopsinic acid)
RN 133695-45-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

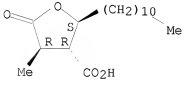
L14 ANSWER 15 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:152994 CAPLUS
DOCUMENT NUMBER: 143:193827
TITLE: Paraconic acids - the natural products from Lichen symbiont
AUTHOR(S): Bandichhor, Rakeshwar; Nosse, Bernd; Reiser, Oliver
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg, 93053, Germany
SOURCE: Topics in Current Chemistry (2005), 243(Natural Product Synthesis I), 43-72
CODEN: TPCCAQ; ISSN: 0340-1022
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Paraconic acids, belonging to the class of γ-butyrolactone natural products, display a broad range of biol. activities such as antibiotic and antitumor properties. Consequently a great number of synthetic strategies have been devised for them, ranging from diastereoselective and chiral pool approaches to the application of asym. catalysis. This review gives a critical account on the different methods developed that lead to paraconic acids of great structural variety.

IT 480-71-7DP, Nephrosteranic acid, derivs. 19464-85-8DP, Roccellaric acid, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthetic strategies for preparation of paraconic acids, natural products from lichen symbiont)

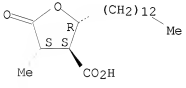
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



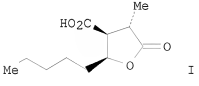
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 136 THERE ARE 136 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

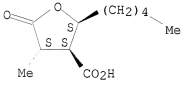
L14 ANSWER 16 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:890611 CAPLUS
DOCUMENT NUMBER: 142:38036
TITLE: A Straightforward Synthesis of (-)-Phaseolinic Acid
AUTHOR(S): Amador, Marta; Ariza, Xavier; Garcia, Jordi; Ortiz, Jordi
CORPORATE SOURCE: Departament de Quimica Organica, Universitat de Barcelona, Barcelona, E-08028, Spain
SOURCE: Journal of Organic Chemistry (2004), 69(23), 8172-8175
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:38036
GI



I

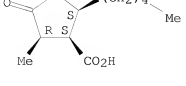
AB A concise approach to (-)-phaseolinic acid (I) starting from com. available (S)-oct-1-yn-3-ol is disclosed. The key steps are a ring-closing metathesis reaction to prepare a C2-sym. allylic diol and its desymmetrization to a γ-butyrolactone by using an Ireland-Claisen rearrangement. The 2S,3S,4S configuration of the levogyre natural product has been confirmed.
IT 109667-12-1P 807346-05-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (-)-phaseolinic acid)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 807346-05-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

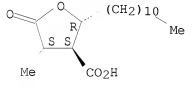
L14 ANSWER 17 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:774780 CAPLUS
DOCUMENT NUMBER: 141:410750
TITLE: Stereoselective synthesis of (+)-nephrosteranic acid, (+)-trans-cognac lactone, and (+)-trans-whisky lactone using a chiral cyclohexadienyl Ti compound
AUTHOR(S): Schleth, Florian; Vogler, Thomas; Harms, Klaus; Studer, Armido
CORPORATE SOURCE: Fachbereich Chemie der Universitaet Marburg, Marburg, 35032, Germany
SOURCE: Chemistry--A European Journal (2004), 10(17), 4171-4185
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:410750

AB We present the stereoselective transfer of cyclohexadienyl from 3-metalated 1,4-cyclohexadienes to various aldehydes. Lewis-acid-mediated "allylation" of aldehydes by treatment with 3-silylated and 3-stannylated 1,4-cyclohexadienes could not be achieved with high diastereoselectivity. In contrast, cyclohexadienyl titanium compds. reacted with both aliphatic and aromatic aldehydes with good-to-excellent diastereoselectivities. Reaction of a chiral TADDOL-derived (TADDOL, 2,2-dimethyl-α,α,α',α'-tetraphenyl-1,3-dioxolandimethanol) cyclohexadienyl Ti derivative with various aldehydes led to the corresponding homoallylic alcs. with excellent diastereo- and enantioselectivities. Lower selectivities were obtained with chiral B-cyclohexadienyldiisopinocampheylborane. The 1,3-cyclohexadienes are very useful building blocks for the preparation of biol. important γ-butyrolactones. Short efficient syntheses of (+)-nephrosteranic acid, (+)-trans-whisky lactone, and (+)-trans-cognac lactone by desymmetrization of 1,4-cyclohexadiene are described.

IT 70579-56-5P, (+)-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of (+)-nephrosteranic acid, (+)-trans-cognac lactone, and (+)-trans-whiskey lactone using a chiral cyclohexadienyl titanium compound)

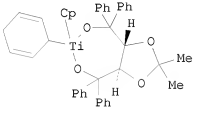
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.

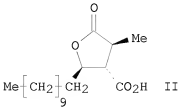


REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 18 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:70305 CAPLUS
DOCUMENT NUMBER: 140:270664
TITLE: Desymmetrization of metalated cyclohexadienes and application to the synthesis of nephrosteranic acid
AUTHOR(S): Schleth, Florian; Studer, Armido
CORPORATE SOURCE: Fachbereich Chemie der Universitaet, Marburg, 35032, Germany
SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 313-315
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:270664
GI



I



II

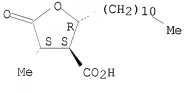
AB Chiral cyclohexadienyl Ti-TADDOLate (I) reacts with aldehydes to provide the corresponding homoallyl alcs. in high yields with excellent diastereo- and high enantioselectivities. The new method has been used as the key step in an efficient synthesis of nephrosteranic acid (II).

IT 70579-56-5P, (+)-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(desymmetrization of metalated cyclohexadienes and application to the synthesis of nephrosteranic acid)

RN 70579-56-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(CA INDEX NAME)

Absolute stereochemistry.



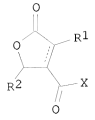
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 19 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:60242 CAPLUS
DOCUMENT NUMBER: 140:111267
TITLE: Preparation of γ-butyrolactone-4-carboxylate derivatives as inhibitors of fatty acid synthase
INVENTOR(S): Kuhadja, Francis P.; Medghalchi, Susan M.; Thupari, Jagan N.; Townsend, Craig A.; McFadden, Jill M.
PATENT ASSIGNEE(S): Fasgen, Llc., USA; The Johns Hopkins University
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004006835	A2	20040122	WO 2003-US20960	20030701
WO 2004006835	A3	20040722		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2491183	A1	20040122	CA 2003-2491183	20030701
AU 2003248810	A1	20040202	AU 2003-248810	20030701
EP 1534263	A2	20050601	EP 2003-764343	20030701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005533107	T	20051104	JP 2004-521521	20030701
CN 1705478	A	20051207	CN 2003-818369	20030701
IN 2004KN02001	A	20070309	IN 2004-KN2001	20041229
US 20060241177	A1	20061026	US 2006-519804	20060519
IN 2008KN02395	A	20090123	IN 2008-KN2395	20080613

PRIORITY APPLN. INFO.:			
	US 2002-392809P	P	20020701
	WO 2003-US20960	W	20030701
	IN 2004-KN2001	A3	20041229

OTHER SOURCE(S): MARPAT 140:111267
GI



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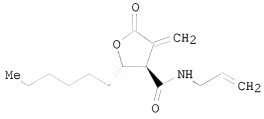


II

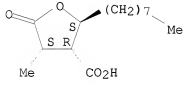
AB The title compds. I [R1 = H, (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.; R2 = (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.; X = OR3 or NHR3, where R3 = H, (cyclo)alkyl, alkenyl, (alkyl)aryl, etc.] were prepared as inhibitors of fatty acid synthase and neuropeptide-Y for weight loss, anti-microbial and anti-cancer applications. Thus, reaction of (±)-α-methylene-γ-butyrolactone-5-hexyl-4-carboxylic acid with allylamine yielded compound II. The latter inhibits human fatty acid synthase with IC50 = 81 μg/mL.

IT 647830-51-1P 647830-52-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of γ-butyrolactone carboxylate derivs. as inhibitors of fatty acid synthase)

RN 647830-51-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4R)-rel- (CA INDEX NAME)

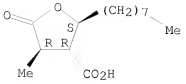
Relative stereochemistry.



RN 647830-52-2 CAPLUS

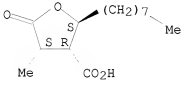
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



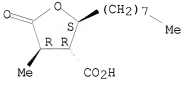
IT 647830-61-3P 647830-62-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of γ-butyrolactone carboxylate derivs. as inhibitors of fatty acid synthase)
RN 647830-61-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4S)-(CA INDEX NAME)

Absolute stereochemistry.



RN 647830-62-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4R)-(CA INDEX NAME)

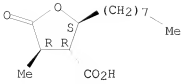
Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

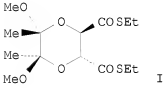
L14 ANSWER 20 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:885658 CAPLUS
DOCUMENT NUMBER: 140:156943
TITLE: Fatty Acid Synthase Inhibition Triggers Apoptosis during S Phase in Human Cancer Cells
AUTHOR(S): Zhou, Weibo; Simpson, P. Jeanette; McFadden, Jill M.; Townsend, Craig A.; Medghalchi, Susan M.; Vadlamudi, Aravinda; Pinn, Michael L.; Ronnett, Gabriele V.; Kuhajda, Francis P.
CORPORATE SOURCE: Department of Pathology, The Johns Hopkins University School of Medicine, Baltimore, MD, 21205, USA
SOURCE: Cancer Research (2003), 63(21), 7330-7337
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB C75, an inhibitor of fatty acid synthase (FAS), induces apoptosis in cultured human cancer cells. Its proposed mechanism of action linked high levels of malonyl-CoA after FAS inhibition to potential downstream effects including inhibition of carnitine palmitoyltransferase-1 (CPT-1) with resultant inhibition of fatty acid oxidation Recent data has shown that C75 directly stimulates CPT-1 increasing fatty acid oxidation in MCF-7 human breast cancer cells despite inhibitory concns. of malonyl-CoA. In light of these findings, we have studied fatty acid metabolism in MCF7 human breast cancer cells to elucidate the mechanism of action of C75. We now report that: (a) in the setting of increased fatty acid oxidation, C75 inhibits fatty acid synthesis; (b) C273, a reduced form of C75, is unable to inhibit fatty acid synthesis and is nontoxic to MCF7 cells; (c) C75 and 5-(tetradecyloxy)-2-furoic acid (TOFA), an inhibitor of acetyl-CoA carboxylase, both cause a significant reduction of fatty acid incorporation into phosphatidylcholine, the major membrane phospholipid, within 2 h; (d) pulse chase studies with [14C]acetate labeling of membrane lipids show that both C75 and TOFA accelerate the decay of 14C-labeled lipid from membranes within 2 h; (e) C75 also promotes a 2-3-fold increase in oxidation of membrane lipids within 2 h; and (f) because interference with phospholipid synthesis during S phase is known to trigger apoptosis in cycling cells, we performed double-labeled terminal deoxynucleotidyltransferase-mediated nick end labeling and BrdUrd anal. with both TOFA and C75. C75 triggered apoptosis during S phase, whereas TOFA did not. Moreover, application of TOFA 2 h before C75 blocked the C75 induced apoptosis, whereas etomoxir did not. Taken together these data indicate that FAS inhibition and its downstream inhibition of phospholipid production is a necessary part of the mechanism of action of C75. CPT-1 stimulation does not likely play a role in the cytotoxic response. The continued ability of TOFA to rescue cancer cells from C75 cytotoxicity implies a proapoptotic role for malonyl-CoA independent of CPT-1 that selectively targets cancer cells as they progress into S phase.
IT 647830-62-4, C 273
RL: PAC (Pharmacological activity); BIOL (Biological study)
(fatty acid synthase inhibition triggers apoptosis during S phase in human cancer cells)
RN 647830-62-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo-, (2S,3R,4R)-(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 21 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:784822 CAPLUS
DOCUMENT NUMBER: 139:395740
TITLE: Aldol Reactions of Dioxanes Derived from Tartaric Acid. A Total Synthesis of (+)-Nephrosteranic Acid
AUTHOR(S): Barros, M. Teresa; Maycock, Christopher D.; Ventura, M. Rita
CORPORATE SOURCE: Instituto de Tecnologia Quimica e Biologica, Universidade Nova de Lisboa, Oeiras, 2781-901, Port.
SOURCE: Organic Letters (2003), 5(22), 4097-4099
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395740
GI



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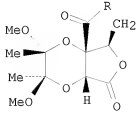


II

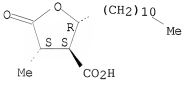
AB A general enantioselective synthesis of the paraconic acids was developed. The key step was a highly stereoselective aldol reaction between a dioxane dithioester I derived from L-tartaric acid and a suitable aldehyde to give lactones II (R = C5H11, C11H23, C13H27).

IT 70579-56-5P, (+)-Nephrosteranic Acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(aldol reactions of dioxanes derived from tartaric acid. in total synthesis of (+)-nephrosteranic acid)

RN 70579-56-5 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

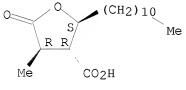
L14 ANSWER 22 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:69772 CAPLUS
DOCUMENT NUMBER: 138:271423
TITLE: Enantioselective synthesis of paraconic acids
AUTHOR(S): Chhor, Rakeshwar B.; Nosse, Bernd; Sorgel, Sebastian; Bohm, Claudius; Seitz, Michael; Reiser, Oliver
CORPORATE SOURCE: Institut fur Organische Chemie Universitat Regensburg, Regensburg, 93053, Germany
SOURCE: Chemistry--A European Journal (2003), 9(1), 260-270
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:271423

AB The development of a new method for the enantioselective synthesis of disubstituted γ-butyrolactones is reported. Based on this strategy, the total synthesis of three paraconic acids, that is (-)-roccellaric acid, (-)-nephrosteranic acid and (-)-protopraesorediosic acid, and the formal total synthesis of (-)-methylenolactocin and (-)-protolichesterinic acid is described, which are important because of their antibiotic and antitumor properties. Key steps of the synthesis are copper(I)-catalyzed asym. cyclopropanations of furans, highly diastereoselective Sakurai allylations, Lewis acid or Lewis base catalyzed retroaldol/lactonization cascades, and ruthenium(II)-catalyzed, intermol. cross metathesis reactions.

IT 480-71-7P 148676-05-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for preparation of disubstituted γ-butyrolactones via asym. cyclopropanation, Sakurai allylation, retroaldol/lactonization, and intramol. cross-metathesis reactions and application to synthesis of paraconic acids)

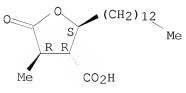
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



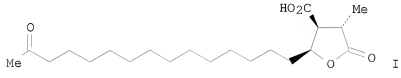
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 23 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:4446 CAPLUS
DOCUMENT NUMBER: 138:237913
TITLE: Synthesis of (±)-nephromopsinic, (-)-phaseolinic, and (-)-dihydropertusaric acids
AUTHOR(S): Brecht-Forster, Andrea; Fitremann, Juliette; Renaud, Philippe
CORPORATE SOURCE: Universite de Fribourg, Departement de Chimie, Fribourg, CH-1700, Switz.
SOURCE: Helvetica Chimica Acta (2002), 85(11), 3965-3974
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237913
GI

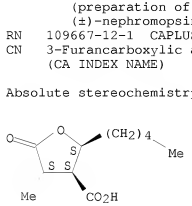


I

AB The formal syntheses of (±)-nephromopsinic acid, (-)-phaseolinic acid, and the first total synthesis of (-)-dihydropertusaric acid (I) from (±)- and (-)-7-oxabicyclo[2.2.1]hept-5-en-2-one are described. These syntheses take advantage of a previously reported radical rearrangement (1,2-acyl migration). A remarkable iodide-mediated cleavage of a bicyclic system, followed by the introduction of the γ-chains via a mixed Kolbe electrolysis, are the key steps of these syntheses. This approach is general and could be applied for the preparation of all kinds of paraconic acids with excellent control of the stereochem.

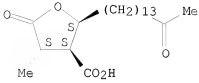
IT 109667-12-1P, (-)-Phaseolinic acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



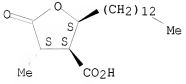
IT 101899-68-7P, (-)-Dihydropertusaric acid 214531-66-5P, (±)-Nephromopsinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)
RN 101899-68-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



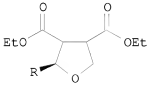
RN 214531-66-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 24 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:4431 CAPLUS
DOCUMENT NUMBER: 138:254998
TITLE: Vicinal dianion of triethyl ethanetricarboxylate: syntheses of (±)-lichesterinic acid, (±)-phaseolinic acid, (±)-nephromopsinic acid, (±)-rocellaric acid, and (±)-dihydroprotolichesterinic acid
AUTHOR(S): Pohmakotr, Manat; Harnying, Wacharee; Tuchinda, Patoomratana; Reutrakul, Vichai
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, 10400, Thailand
SOURCE: Helvetica Chimica Acta (2002), 85(11), 3792-3813
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:254998
GI



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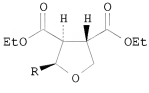


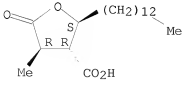
II

AB The vicinal dianion derived from tri-Et ethanetricarboxylate reacted regioselectively with aldehydes and ketones at C(β) to provide paraconic acid derivs. I [R = 4-MeOC6H4, Me3C, Me(CH2)4, etc.] in moderate to high yields as mixts. of diastereoisomers. The paraconic acid derivs. II [R = Me(CH2)n, n = 4, 12] were utilized as the starting materials for the syntheses of (±)-lichesterinic acid, (±)-phaseolinic acid, (±)-nephromopsinic acid, (±)-rocellaric acid, and (±)-dihydroprotolichesterinic acid.

IT 220379-59-9P, (±)-Rocellaric acid 502696-27-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (±)-lichesterinic acid, (±)-phaseolinic acid, (±)-nephromopsinic acid, (±)-rocellaric acid, and (±)-dihydroprotolichesterinic acid from γ-lactones derived from lactonization of carbonyl compds. with tri-Et ethanetricarboxylate)

RN 220379-59-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

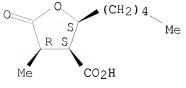
Relative stereochemistry.



RN 502696-27-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-,

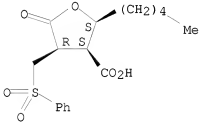
(2R,3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



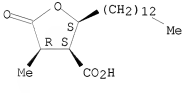
IT 502696-26-6P 502696-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (±)-lichesterinic acid, (±)-phaseolinic acid, (±)-nephromopsinic acid, (±)-rocellaric acid, and (±)-dihydroprotolichesterinic acid from γ-lactones derived from lactonization of carbonyl compds. with tri-Et ethanetricarboxylate)
RN 502696-26-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-5-oxo-2-pentyl-4-[(phenylsulfonyl)methyl]-, (2R,3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



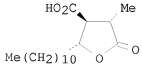
RN 502696-28-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

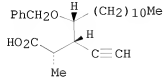


REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 25 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:34084 CAPLUS
DOCUMENT NUMBER: 136:294668
TITLE: Enantioselective syntheses of (+)- and (-)-nephrosteranic acid employing the Nicholas-Schreiber reaction
AUTHOR(S): Jacobi, Peter A.; Herradura, Prudencio
CORPORATE SOURCE: Dep. Chem., Dartmouth College, Hanover, NH, 03755, USA
SOURCE: Canadian Journal of Chemistry (2001), 79(11), 1727-1735
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:294668
GI



I

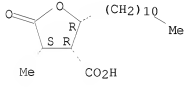


II

AB (+)- And (-)-Nephrosteranic acid (I) have been prepared in an enantioselective fashion from alkyne acid II (or ent-II) by a three step sequence involving debenzylation-lactonization, oxidative cleavage, and selective epimerization at C4. Acids II and ent-II were obtained as single enantiomers employing a Nicholas-Schreiber reaction.

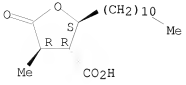
IT 405552-35-4P, (+)-4-epi-Nephrosteranic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective syntheses of (+)- and (-)-nephrosteranic acid via the Nicholas-Schreiber reaction)
RN 405552-35-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3R,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



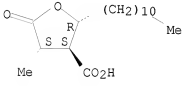
IT 480-71-7P, (-)-Nephrosteranic acid 70579-56-5P, (+)-Nephrosteranic acid 407635-98-7P, (-)-4-epi-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective syntheses of (+)- and (-)-nephrosteranic acid via the Nicholas-Schreiber reaction)
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



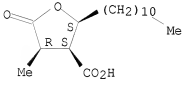
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-
(CA INDEX NAME)

Absolute stereochemistry.



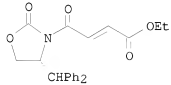
RN 407635-98-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3S,4R)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 26 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:14878 CAPLUS
DOCUMENT NUMBER: 136:247437
TITLE: Free-radical-mediated conjugate additions. enantioselective synthesis of butyrolactone natural products: (-)-enterolactone, (-)-arctigenin, (-)-isoarctigenin, (-)-nephrosteranic acid, and (-)-roccellaric acid
AUTHOR(S): Sibi, Mukund P.; Liu, Pingrong; Ji, Jianguo; Hajra, Saumen; Chen, Jian-xie
CORPORATE SOURCE: Department of Chemistry, North Dakota State University, Fargo, ND, 58105-5516, USA
SOURCE: Journal of Organic Chemistry (2002), 67(6), 1738-1745
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:247437
GI



I

II

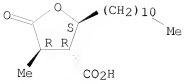
AB Lewis acid-mediated conjugate addition of alkyl radicals to a differentially protected fumarate I produced the monoalkylated succinates with high chemical efficiency and excellent stereoselectivity. A subsequent alkylation or an aldol reaction furnished the disubstituted succinates with syn configuration. The chiral auxiliary, 4-diphenylmethyl-2-oxazolidinone, controlled the stereoselectivity in both steps. Manipulation of the disubstituted succinates obtained by alkylation furnished the natural products (-)-enterolactone, (-)-arctigenin, and (-)-isoarctigenin. The overall yields for the target natural products were 20-26% over six steps. Selective functionalization of the disubstituted succinates obtained by aldol condensation gave the paraconic acid natural products (-)-nephrosteranic acid (II; R = C11H23) and (-)-roccellaric acid (II; R = C13H27). The overall yield of the natural products II over four steps was 53% and 42%, resp.

IT 480-71-7P, (-)-Nephrosteranic Acid 148676-05-5P, (-)-Roccellaric Acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(free-radical-mediated conjugate addns. in enantioselective synthesis of butyrolactone-containing natural products)

RN 480-71-7 CAPLUS

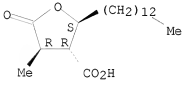
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



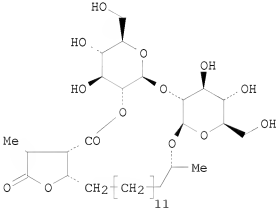
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 27 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:883604 CAPLUS
DOCUMENT NUMBER: 136:229116
TITLE: Macrolactone glycosides of three lichen acids from Acarospora gobiensis, a lichen of Central Asia
AUTHOR(S): Rezanka, Tomas; Guschina, Irina A.
CORPORATE SOURCE: Institute of Microbiology, Prague, 14220, Czech Rep.
SOURCE: Phytochemistry (2001), 58(8), 1281-1287
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

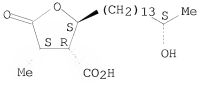
AB The compds. isolated from the extract of Central Asian lichen (Acarospora gobiensis H. Magn.) comprised three new glycosides having 18-hydroxy-dihydroalloprotolichesterinic, 18-hydroxy-neodihydroprotolichesterinic and 18-hydroxy-dihydroprotolichesterinic acids as aglycons and a di- or trisaccharide moiety linked at C-18 and at the carboxylic group. These compds., called gobienines A-C (e.g I, gobienine A), were found to be di- or trisaccharides forming a macrolactone with the aglycon. The structures were elucidated by using extensive spectroscopic anal. (1D and 2D NMR, MS, IR and ORD) and chemical and enzymic methods.

IT 379224-47-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(18S-hydroxydihydroprotolichesterinic acid; gobienine B hydrolysis product)

RN 379224-47-2 CAPLUS

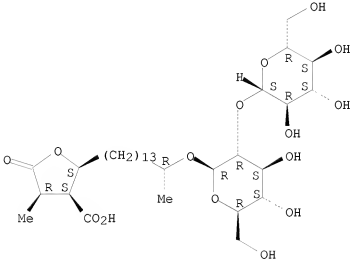
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



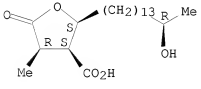
IT 403618-80-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(gobienine A esterase treatment product)
RN 403618-80-4 CAPLUS
CN 3-Furancarboxylic acid, 2-[(14R)-14-[(2-O-β-D-glucopyranosyl-β-D-glucopyranosyl)oxy]pentadecyl]tetrahydro-4-methyl-5-oxo-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



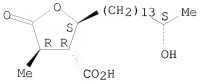
IT 379224-46-1P, 18R-Hydroxydihydroalloprotolichesterinic acid
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(gobienine A hydrolysis product)
RN 379224-46-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



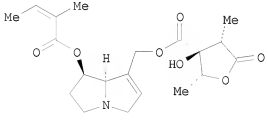
IT 379224-48-3P, 18S-Hydroxyneodihydroprotolichesterinic acid
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(gobienine B hydrolysis product)
RN 379224-48-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 28 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:697552 CAPLUS
DOCUMENT NUMBER: 136:37806
TITLE: Reactive enols in synthesis. 2. Synthesis of (+)-latifolic Acid and (+)-latifoline
AUTHOR(S): Drutu, Ioana; Krygowski, Evan S.; Wood, John L.
CORPORATE SOURCE: Department of Chemistry, Yale University Sterling Chemistry Laboratory, New Haven, CT, 06520-8107, USA
SOURCE: Journal of Organic Chemistry (2001), 66(21), 7025-7029
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:37806
GI



I

II

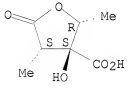
AB The authors describe a short, enantioselective synthesis of the naturally occurring pyrrolizidine alkaloid (+)-latifoline (I) employing a tandem [3,3] sigmatropic rearrangement/[1,2] allyl shift as a key step in constructing (+)-latifolic acid (II).

IT 50460-94-1P, (+)-Latifolic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of (+)-latifoline and (+)-latifolic acid via sigmatropic rearrangement/allyl shift)

RN 50460-94-1 CAPLUS

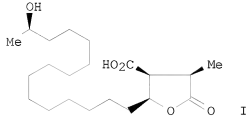
CN L-threo-Pentonic acid, 3-C-carboxy-2,5-dideoxy-2-C-methyl-, γ-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

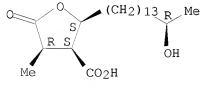
L14 ANSWER 29 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:667445 CAPLUS
DOCUMENT NUMBER: 136:17754
TITLE: Glycoside esters from lichens of central Asia
AUTHOR(S): Rezanka, T.; Guschina, I. A.
CORPORATE SOURCE: Institute of Microbiology, Prague, 14220, Czech Rep.
SOURCE: Phytochemistry (2001), 58(3), 509-516
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

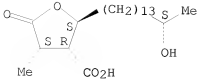
AB Ten compds. (e.g. I) isolated from the extract of the central Asian lichens comprised new glycosides and glycoside esters having 18R-hydroxy-dihydroalloprotolichesterinic, 18S-hydroxy-dihydroprotolichesterinic and 18S-hydroxy-neodihydroprotolichesterinic acids, as the aglycons and a saccharide moiety linked at C-18 and also at C-21 made by glucose, xylose or rhamnose. The structures were elucidated using extensive spectroscopic anal. (1D and 2D NMR, MS, IR, UV and ORD) and by biochem. methods.
IT 379224-46-1P, 18R-Hydroxydihydroalloprotolichesterinic acid
379224-47-2P, 18S-Hydroxydihydroprotolichesterinic acid
379224-48-3P, 18S-Hydroxyneodihydroprotolichesterinic acid
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(glycoside esters from lichens of central Asia)
RN 379224-46-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



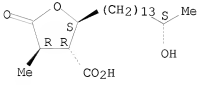
RN 379224-47-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 379224-48-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14S)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

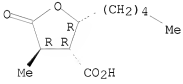
L14 ANSWER 30 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:321140 CAPLUS
DOCUMENT NUMBER: 135:107173
TITLE: A concise synthesis of (±)-methylenolactocin and the formal synthesis of (±)-phaseolinic acid
AUTHOR(S): Loh, T.-P.; Lye, P.-L.
CORPORATE SOURCE: Department of Chemistry, The National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2001), 42(20), 3511-3514
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:107173

AB (±)-Methylenolactocin was prepared in five steps involving an indium-mediated allylation reaction as the key step.

IT 203514-35-6P, (±)-Phaseolinic acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(synthesis of (±)-methylenolactocin and formal synthesis of (±)-phaseolinic acid via indium-mediated allylation)

RN 203514-35-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

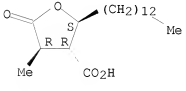
L14 ANSWER 31 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:238464 CAPLUS
DOCUMENT NUMBER: 135:33403
TITLE: Enantioselective Synthesis of (-)-Roccellaric Acid
AUTHOR(S): Boehm, Claudius; Reiser, Oliver
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg, 93053, Germany
SOURCE: Organic Letters (2001), 3(9), 1315-1318
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:33403

AB A new strategy for the synthesis of anti-4,5-disubstituted γ-butyrolactones starting from inexpensive furan-2-carboxylic Me ester was developed. By applying this methodol., the enantioselective synthesis of (-)-roccellaric acid was accomplished using a copper(I)-catalyzed asym. cyclopropanation, a tin(IV)-catalyzed retroaldol/lactonization sequence of cyclopropanols, and a ruthenium-catalyzed intermol. metathesis reaction as key steps.

IT 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of the γ-butyrolactone (-)-roccellaric acid)

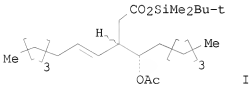
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 32 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:61277 CAPLUS
DOCUMENT NUMBER: 134:252178
TITLE: A concise synthesis of (−)-methylenolactocin and (−)-phaseolinic acid from (6S,9S)-tetradec-7-yne-6,9-diol
AUTHOR(S): Ariza, Xavier; Garcia, Jordi; Lopez, Marta; Montserrat, Laia
CORPORATE SOURCE: Departament de Quimica Organica, Div. III, Universitat de Barcelona, Barcelona, 08028, Spain
SOURCE: Synlett (2001), (1), 120-122
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:252178
GI



I

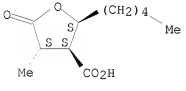
AB A novel, stereodivergent route to paraconic acids from C2-sym. trans- and cis-alk-2-ene-1,4-diols through Ireland-Claisen and/or Johnson ortho ester I (threo = β-H; erythro = α-H) rearrangements was accomplished. This strategy was applied to the synthesis of (−)-methylenolactocin and (−)-phaseolinic acid from the chiral title diol.

IT 109667-12-1P, (−)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (−)-methylenolactocin and (−)-phaseolinic acid from (6S,9S)-tetradec-7-yne-6,9-diol)

RN 109667-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

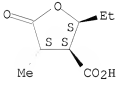
Absolute stereochemistry. Rotation (−).



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

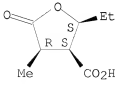
L14 ANSWER 33 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:605272 CAPLUS
DOCUMENT NUMBER: 134:4544
TITLE: Configurational assignments of diastereomeric γ-lactones using vicinal H-H NMR coupling constants and molecular modeling
AUTHOR(S): Stortz, Carlos A.; Maier, Marta S.
CORPORATE SOURCE: Facultad de Ciencias Exactas y Naturales, Departamento de Quimica Organica, Universidad de Buenos Aires, Buenos Aires, 1428, Argent.
SOURCE: Perkin 2 (2000), (9), 1832-1836
CODEN: PRKTFO; ISSN: 1470-1820
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The conformational features of four diastereomers of the γ-lactone, 2-ethyl-4-methyl-5-oxotetrahydrofuran-3-carboxylic acid, were investigated by calcns. which included mol. mechanics (MM3), semiempirical (AM1) and ab initio MO theory (HF/6-31G), the latter including solvent emulation. Results were compared with those obtained by 1H NMR spectroscopy of natural and synthetic analogs in which a long aliphatic chain replaces the Et side chain. A notable agreement was found between the exptl. vicinal ring coupling consts. and those computed by the ab initio calcn.; MM3 also gave rise to a fair agreement, while AM1 shows large failures to encounter the potential energy surface of these and other five-membered rings.
IT 307984-44-7 307984-46-9 307984-48-1
307984-50-5
RL: PRP (Properties)
(configurational assignments of diastereomeric γ-lactones using vicinal H-H NMR coupling consts. and mol. modeling)
RN 307984-44-7 CAPLUS
CN 3-Furancarboxylic acid, 2-ethyltetrahydro-4-methyl-5-oxo-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.



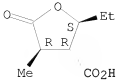
RN 307984-46-9 CAPLUS
CN 3-Furancarboxylic acid, 2-ethyltetrahydro-4-methyl-5-oxo-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



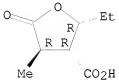
RN 307984-48-1 CAPLUS
CN 3-Furancarboxylic acid, 2-ethyltetrahydro-4-methyl-5-oxo-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 307984-50-5 CAPLUS
CN 3-Furancarboxylic acid, 2-ethyltetrahydro-4-methyl-5-oxo-, (2R,3R,4R)-
(CA INDEX NAME)

Absolute stereochemistry.



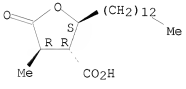
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 34 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:85990 CAPLUS
DOCUMENT NUMBER: 132:236929
TITLE: Asymmetric carbolithiation of 2-phenylselenofumarate derivatives: a short synthesis of (-)-roccellaric acid
AUTHOR(S): Bella, Marco; Margarita, Roberto; Orlando, Claudia; Orsini, Monica; Parlanti, Luca; Piancatelli, Giovanni
CORPORATE SOURCE: Dipartimento di Chimica, Universita "La Sapienza", Rome, 00185, Italy
SOURCE: Tetrahedron Letters (2000), 41(4), 561-565
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:236929

AB (-)-Roccellaric acid and variously substituted succinates are obtained through direct asym. carbolithiation of 2-phenylselenofumarate derivs., followed by reaction with suitable electrophiles.

IT 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (-)-roccellaric acid via asym. carbolithiation of 2-phenylselenofumarate derivs.)
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

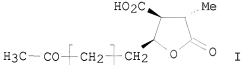
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 35 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:665856 CAPLUS
DOCUMENT NUMBER: 132:33194
TITLE: A Revised Structure for (-)-Dihydropertusaric Acid, a γ-Butyrolactone Acid from the Lichen Punctelia microsticta
AUTHOR(S): Maier, Marta S.; Gonzalez Marimon, Diego I.; Stortz, Carlos A.; Adler, Monica T.
CORPORATE SOURCE: Departamento de Química Organica and Departamento de Ciencias Biologicas, Facultad de Ciencias Exactas y Naturales, Buenos Aires, 1428, Argent.
SOURCE: Journal of Natural Products (1999), 62(11), 1565-1567
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

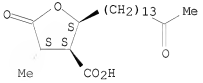


AB The γ-butyrolactone acid, (-)-dihydropertusaric acid (I), and two known compds., (-)-isomuronic acid and the tridepside gyrophoric acid, were isolated from the lichen Punctelia microsticta. The structure and stereochem. of I were determined on the basis of spectroscopic evidence and mol. modeling. Spectroscopic and phys. data of I were identical with those of a previously isolated compound from the lichen Pertusaria albescens which had been reported with a different relative configuration.

IT 101899-68-7P, (-)-Dihydropertusaric acid
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
(isolation, mol. structure, conformation, and revised configuration for (-)-dihydropertusaric acid, a γ-butyrolactone acid from the lichen Punctelia microsticta)

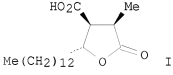
RN 101899-68-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 36 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:602818 CAPLUS
DOCUMENT NUMBER: 131:336854
TITLE: Total synthesis of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid by radical cyclization of an epoxide using a transition-metal radical source
AUTHOR(S): Mandal, Pijus Kumar; Roy, Subhas Chandra
CORPORATE SOURCE: Department of Organic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700032, India
SOURCE: Tetrahedron (1999), 55(37), 11395-11398
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:336854
GI

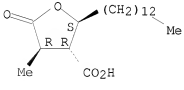


I

AB A short and efficient total synthesis of (±)-dihydroprotolichesterinic acid (I) and the formal synthesis of (±)-rocellaric acid were achieved by radical cyclization of an epoxide using a transition metal radical source.

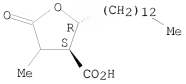
IT 220379-59-9P, (±)-Rocellaric acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)
RN 220379-59-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



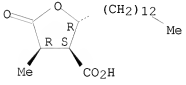
IT 249647-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)
RN 249647-94-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



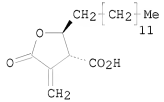
IT 249921-70-8P, (±)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (±)-dihydroprotolichesterinic acid and formal synthesis of (±)-rocellaric acid via intramol. titanium radical cyclization)
RN 249921-70-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

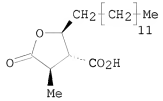


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 37 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:811697 CAPLUS
DOCUMENT NUMBER: 130:168148
TITLE: Efficient total syntheses of (±)protolichesterinic acid and (±)rocellaric acid via tungsten-π-allyl complexes
AUTHOR(S): Chen, Ming-Jung; Liu, Rai-Shung
CORPORATE SOURCE: Department of Chemistry, National Tsing Hua University, Hsinchu, 30043, Taiwan
SOURCE: Tetrahedron Letters (1998), 39(51), 9465-9468
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:168148
GI



I



II

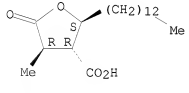
AB Total syntheses of racemic protolichesterinic acid (I) and rocellaric acid (II) were achieved with the use of tungsten-π-allyl complex in the key step. I and II were prepared in four and six steps resp. starting from readily available chloropropargyl derivs.

IT 220379-59-9P, (±)-Rocellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(total syntheses of (±)-protolichesterinic acid and (±)-rocellaric acid via tungsten-π-allyl complexes)

RN 220379-59-9 CAPLUS

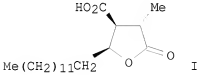
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 38 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:603556 CAPLUS
DOCUMENT NUMBER: 129:302486
ORIGINAL REFERENCE NO.: 129:61703a,61706a
TITLE: Synthesis of (±)-nephromopsinic acid
AUTHOR(S): Forster, Andrea; Fitremann, Juliette; Renaud, Philippe
CORPORATE SOURCE: Institut de Chimie Organique, Universite de Fribourg, Fribourg, 1700, Switz.
SOURCE: Tetrahedron Letters (1998), 39(39), 7097-7100
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:302486
GI



I

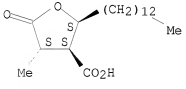
AB The preparation of (±)-nephromopsinic acid (I) form 7-oxabicyclo[2.2.1]hept-5-en-2-one is reported. The synthesis takes advantage of a previously reported radical acyl migration. A remarkable iodide mediated cleavage of the bicyclic systems followed by the introduction of the γ-chain via a mixed Kolbe electrolysis are the key features of this approach. This strategy is expected to be of interest for the preparation of all kinds of paraconic acids with excellent control of the stereochem.

IT 214531-66-5P, (±)-Nephromopsinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (±)-nephromopsinic acid)

RN 214531-66-5 CAPLUS

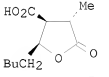
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

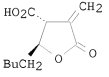


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

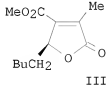
L14 ANSWER 39 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:169746 CAPLUS
DOCUMENT NUMBER: 128:204723
ORIGINAL REFERENCE NO.: 128:40487a,40490a
TITLE: Synthesis of (+)- and (-)-Phaseolinic Acid by Combination of Enzymic Hydrolysis and Chemical Transformations with Revision of the Absolute Configuration of the Natural Product
AUTHOR(S): Drioli, Sara; Felluga, Fulvia; Forzato, Cristina; Nitti, Patrizia; Pitacco, Giuliana; Valentin, Ennio
CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita, Trieste, 34127, Italy
SOURCE: Journal of Organic Chemistry (1998), 63(7), 2385-2388
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:204723
GI



I



II



III

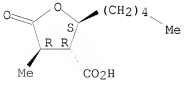
AB Synthesis of both enantiomers of phaseolinic acid and on the determination of their absolute configurations via chemical and spectroscopic correlations is reported. The strategy was to correlate (-)-phaseolinic acid (I) with (-)-methylenolactocin (II) through the butenolide III.

IT 203864-73-7P
RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(absolute configuration of phaseolinic acid enantiomers via stereoselective synthesis)

RN 203864-73-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



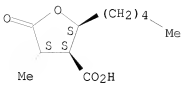
IT 109667-12-1P 185246-65-5P
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(absolute configuration of phaseolinic acid enantiomers via stereoselective synthesis)

RN 109667-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)-

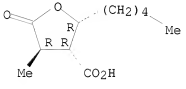
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



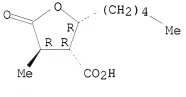
RN 185246-65-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 203514-35-6P, (±)-Phaseolinic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(absolute configuration of phaseolinic acid enantiomers via stereoselective
synthesis)
RN 203514-35-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-,
(2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

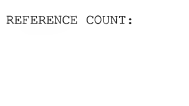
L14 ANSWER 40 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:521418 CAPLUS
DOCUMENT NUMBER: 127:176567
ORIGINAL REFERENCE NO.: 127:34211a,34214a
TITLE: Exerting face-stereoselective shielding: design of an enantiomeric pair of camphene-based oxazolidin-2-ones for use as recyclable chiral auxiliaries in asymmetric synthesis
AUTHOR(S): Cadogan, J. I. G.; Doyle, A. A.; Gosney, I.; Hodgson, P. K. G.; Thorburn, P.
CORPORATE SOURCE: Department of Chemistry, Imperial College of Science, Technology and Medicine, London, SW7 2AY, UK
SOURCE: Enantiomer (1997), 2(2), 81-98
CODEN: EANTE2; ISSN: 1024-2430
PUBLISHER: Gordon & Breach
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 17 refs. Preparative methodol. is described for access to a range of enantiomerically pure oxazolidin-2-ones by chemical elaboration of naturally-occurring compds. (terpenes, carbohydrates) via a stereospecific intramol. nitrene insertion reaction. The effectiveness and limitations of these reagents as chiral control elements in the form of their N-acyl derivs. for an array of asym. transformations is reported. In particular, the efficiency of a (+)-spiro-oxazolidin-2-one obtained from (-)-camphene is highlighted by the virtually complete stereoselection attained in such reactions as the Diels-Alder, conjugate addition, aldol, alkylation and acylation reactions. An added benefit to the spiro-oxazolidin-2-one is that its (-)-enantiomer is also readily accessible from (+)-camphene, thereby allowing preparative access to both enantiomeric products in a range of asym. manipulations. Both reagents are readily cleaved from the newly created chiral moieties and can be recycled. This exceptional quality of asym. induction imparted by the (+)-spiro-oxazolidin-2-one is highlighted by a concise synthesis of the tri-substituted lactone (-)-dihydroprotolichesterinic acid in 57% overall yield via consecutive stereo-controlled 1,4-conjugate addition and syn-aldol reactions.

IT 144356-39-8P, (-)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(design of enantiomeric pair of camphene-based oxazolidin-2-ones for use as recyclable chiral auxiliaries in asym. synthesis)

RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

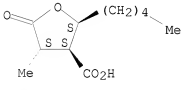
Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

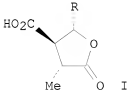
L14 ANSWER 41 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:343886 CAPLUS
DOCUMENT NUMBER: 127:50457
ORIGINAL REFERENCE NO.: 127:9625a,9628a
TITLE: Asymmetric resolution of diastereomeric 4-ethoxycarbonyl-5-pentyl-γ-butyrolactones by crude PLE-mediated hydrolysis
AUTHOR(S): Drioli, Sara; Felluga, Fulvia; Forzato, Cristina; Nitti, Patrizia; Pitacco, Giuliana; Valentin, Ennio
CORPORATE SOURCE: Dipartimento di Scienze Chimiche, Universita di Trieste, via L. Giorgieri 1, Trieste, I-34127, Italy
SOURCE: Journal of Molecular Catalysis B: Enzymatic (1997), 3(1-4), 203-207
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50457
AB Chemical reduction of di-Et 1-oxo-hexylsuccinate resulted in the formation of the corresponding cis and trans-disubstituted γ-butyrolactones. Both racemic diastereomers were resolved by means of lipolytic enzymes leading to the precursors of interesting natural products such as (-)-methylenolactocin and (-)-phaseolinic acid.
IT 109667-12-1P, (-)-Phaseolinic acid
RL: PNU (Preparation, unclassified); PREP (Preparation)
(asym. resolution of diastereomeric 4-ethoxycarbonyl-5-pentyl-γ-butyrolactones by crude PLE-mediated hydrolysis)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

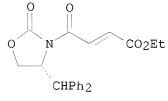


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 42 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:142049 CAPLUS
DOCUMENT NUMBER: 126:211956
ORIGINAL REFERENCE NO.: 126:40987a,40990a
TITLE: Regio- and stereocontrolled conjugate radical addition to a desymmetrized fumarate derivative: an efficient synthesis of (-)-nephrosteranic acid and (-)-roccellaric acid
AUTHOR(S): Sibi, Mukund P.; Ji, Jianguo
CORPORATE SOURCE: Dep. Chem., North Dakota State Univ., Fargo, ND, 58105-5516, USA
SOURCE: Angewandte Chemie, International Edition in English (1997), 36(3), 274-276
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:211956
GI



I



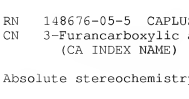
II

AB (-)-Nephrosteranic acid (I, R = C11H23) and (-)-roccellaric acid (I, R = C13H27) were prepared via high regio- and diastereoselective addition of the desymmetrized fumarate II with C1CH2I mediated by Samarium triflate.

IT 480-71-7P, (-)-Nephrosteranic acid 148676-05-5P, (-)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereocontrolled conjugate radical addition to a desymmetrized fumarate derivative in synthesis of (-)-nephrosteranic acid and (-)-roccellaric acid)

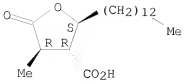
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

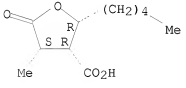
L14 ANSWER 43 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:711181 CAPLUS
DOCUMENT NUMBER: 126:59779
ORIGINAL REFERENCE NO.: 126:11737a,11740a
TITLE: Enantioselective syntheses of (+)- and (-)-phaseolinic acid
AUTHOR(S): Jacobi, Peter A.; Herradura, Prudencio
CORPORATE SOURCE: Hall-Atwater Lab., Wesleyan Univ., Middletown, CT, 06459-0180, USA
SOURCE: Tetrahedron Letters (1996), 37(46), 8297-8300
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (+)- And (-)-Phaseolinic acid have been prepared in an enantioselective fashion from (2S,3S,4R)-HO2CCHMeCH(C.tplbond.CH)CH(OCH2Ph)(CH2)4Me (I) by a three-step sequence involving lactonization, epimerization at C-3, and oxidative cleavage. I was obtained as a single enantiomer using a Nicholas-Schreiber reaction.

IT 185246-78-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective syntheses of (+)- and (-)-phaseolinic acid)

RN 185246-78-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4S)- (CA INDEX NAME)

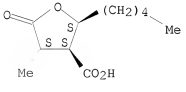
Absolute stereochemistry.



IT 109667-12-1P, (-)-Phaseolinic acid 185246-58-6P
185246-60-0P 185246-65-5P, (+)-Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective syntheses of (+)- and (-)-phaseolinic acid)

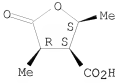
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



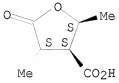
RN 185246-58-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2,4-dimethyl-5-oxo-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



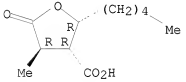
RN 185246-60-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2,4-dimethyl-5-oxo-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.



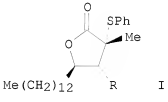
RN 185246-65-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 44 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:501492 CAPLUS
DOCUMENT NUMBER: 125:167635
ORIGINAL REFERENCE NO.: 125:31409a,31412a
TITLE: Efficient Stereoselective Synthesis of the Enantiomers of Highly Substituted Paraconic Acids
AUTHOR(S): Martin, Tomas; Rodriguez, Carmen M.; Martin, Victor S.
CORPORATE SOURCE: Instituto Universitario de Bio-Organica Antonio Gonzalez, Universidad de La Laguna, La Laguna, 38206, Spain
SOURCE: Journal of Organic Chemistry (1996), 61(18), 6450-6453
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

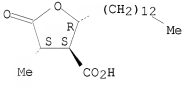
AB Rocellaric, protolichesterinic and dihydroprotolichesterinic acids were prepared stereoselectively via the common α-phenylthio-γ-lactone I [R = CH2CO2Me], obtained by a previously reported methodol. The described syntheses are general for this class of compds. The key steps are the conversion of the I [R = CH2CO2Me] to I [R = CO2H] with cleavage of one carbon, via I [R = CH(OH)CH2OH], and stereochem. controlled removal of the PhS group.

IT 19464-85-8P 19464-87-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of paraconic acids)

RN 19464-85-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

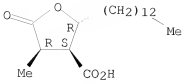
Absolute stereochemistry. Rotation (+).



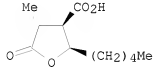
RN 19464-87-0 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

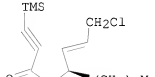
Absolute stereochemistry.


O
O
R
R S
(CH2)12
Me
Me
CO2H

L14 ANSWER 45 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:465659 CAPLUS
DOCUMENT NUMBER: 125:195252
ORIGINAL REFERENCE NO.: 125:36563a,36566a
TITLE: Total synthesis of phaseolinic acid by enyne cyclization
AUTHOR(S): Zhang, Zhaoguo; Lu, Xiyan
CORPORATE SOURCE: Shanghai Inst. of Organic Chemistry, Chinese Acad. of Sci., Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (1996), 7(7), 1923-1928
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:195252
GI



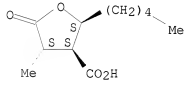
I



II

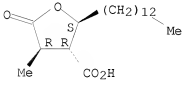
AB Enantiopure phaseolinic acid I was synthesized from (R)-4'-chloro-1'-n-pentyl-2'-butenyl 3-trimethylsilyl-2-propynoate II by palladium(II) catalyzed cyclization reaction as the key step.
IT 109667-12-1P, Phaseolinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of phaseolinic acid via palladium(II) catalyzed enyne cyclization)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

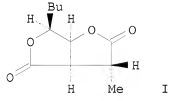


L14 ANSWER 46 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:274723 CAPLUS
DOCUMENT NUMBER: 125:10426
ORIGINAL REFERENCE NO.: 125:2293a,2296a
TITLE: Regio- and stereoselective functionalization of linear dicarboxylic acid derivatives. A sequential aldol-lactonization strategy for the synthesis of (-)-roccellaric acid, (-)-protolichesterinic acid, and (-)-methylenolactocin
AUTHOR(S): Sibi, Mukund P.; Deshpande, Prasad K.; La Loggia, Anthony J.
CORPORATE SOURCE: Dep. of Chemistry, North Dakota State Univ., Fargo, ND, 58105-5516, USA
SOURCE: Synlett (1996), (4), 343-345
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A regio- and stereoselective functionalization methodol. for linear dicarboxylic acids has been developed and applied in the synthesis of paraconic acid natural products. Using this strategy, (-)-roccellaric acid was prepared in 25% overall yield and 4 steps from a differentially functionalized succinate. The formal total synthesis of (-)-protolichesterinic acid and (-)-methylenolactocin was also accomplished starting from the differentially functionalized succinate.
IT 148676-05-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of paraconic acids)
RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

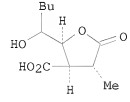
Absolute stereochemistry. Rotation (-).



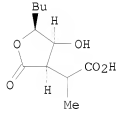
L14 ANSWER 47 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:867525 CAPLUS
DOCUMENT NUMBER: 124:116415
ORIGINAL REFERENCE NO.: 124:21681a,21684a
TITLE: Rates and mechanisms for the ring opening, ring closure and ring transformation reactions of the di-γ-lactone dihydrocanadensolide (DHC)
AUTHOR(S): Aldridge, David C.; Nicholson, Stuart; Taylor, Peter J.
CORPORATE SOURCE: Zeneca Pharmaceuticals, Alderley Park, Macclesfield, Cheshire, SK10 4TG, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1995), (10), 1929-38
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



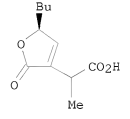
I



II



III

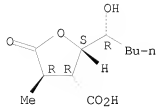


IV

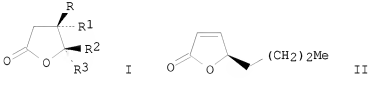
AB The title di-γ-lactone I ring opens in alkali to the monolactones II, III, IV by three parallel routes: via hydrolysis to II and III and via β-elimination to give IV. The last is probably in (E1cb)I process, though there is conflicting evidence and the mechanism is uncertain. The two hydrolyses are much faster than models would predict owing essentially to the ΔS.thermod. term, and an unusual intramol. interaction which results from steric crowding is invoked. While further hydrolysis of the monolactone III is straightforward, that of II probably goes via a δ-lactone , whose rapid pre-equilibration with II has also been studied. This hydrolysis is characterized by a highly abnormal near-zero ΔS.thermod. value which is tentatively explained as being due to exclusion of water from the transition state by intramol. solvation. Rates for the reverse lactonization process are unremarkable, but anal. of the activation parameters reveals evidence for ring strain in the formation of I which precisely balances the normal rate increase expected through approximation
IT 172821-07-7P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(ring opening ring closure and ring transformation reactions of the di-γ-lactone dihydrocanadensolide)
RN 172821-07-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(S*),3α,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L14 ANSWER 48 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:746705 CAPLUS
DOCUMENT NUMBER: 123:143520
ORIGINAL REFERENCE NO.: 123:25557a,25560a
TITLE: Concise Syntheses of Natural γ-Butyrolactones, (+)-trans-Whisky Lactone, (+)-trans-Cognac Lactone, (-)-Methylenolactocin, (+)-Nephrosteranic Acid, and (+)-Roccellaric Acid Using Novel Chiral Butenolide Synthons
AUTHOR(S): Takahata, Hiroki; Uchida, Yasuhiro; Momose, Takefumi
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Toyama Medical Pharmaceutical University, Toyama, 930-01, Japan
SOURCE: Journal of Organic Chemistry (1995), 60(17), 5628-33
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:143520
GI

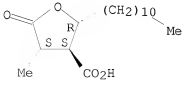


AB Cis-4-Hydroxy-5-(iodomethyl)-4,5-dihydro-2(3H)-furanones I (R = OH, R1 = R3 = H, R2 = CH2I; R = R2 = H, R1 = OH, R3 = CH2I) were converted by cross-coupling with several Grignard-derived cuprates followed by benzoylation and base-induced elimination into new chiral butenolides, e.g., II. The sequential conjugate addition-quenching of these butenolides under complete stereocontrol provided several polysubstituted γ-butyrolactones including flavor components [(+)-trans-whisky lactone and (+)-trans-cognac lactone], the antitumor antibiotic lactone (-)-methylenolactocin, and lichen components [(+)-nephrosteranic acid and (+)-roccellaric acid].

IT 70579-56-5P, (+)-Nephrosteranic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of whisky and cognac lactones, methylenolactocin, nephrosteranic and roccellaric acids)

RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)- (CA INDEX NAME)

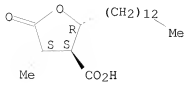
Absolute stereochemistry.



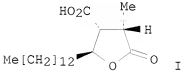
IT 19464-85-8P, (+)-Roccellaric acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of whisky and cognac lactones, methylenolactocin, nephrosteranic and roccellaric acids)

RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-
(CA INDEX NAME)

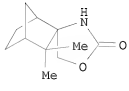
Absolute stereochemistry. Rotation (+).



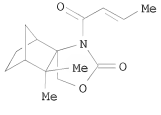
L14 ANSWER 49 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:597893 CAPLUS
DOCUMENT NUMBER: 123:83088
ORIGINAL REFERENCE NO.: 123:14865a,14868a
TITLE: A concise synthesis of (-)-dihydroprotolichesterinic acid via consecutive stereocontrolled 1,4-conjugate addition and syn-aldol condensation reactions
AUTHOR(S): Banks, Malcolm R.; Dawson, Ian M.; Gosney, Ian; Hodgson, Philip K. G.; Thorburn, Paul
CORPORATE SOURCE: Dep. of Chemistry, The University of Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Tetrahedron Letters (1995), 36(20), 3567-70
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:83088
GI



I



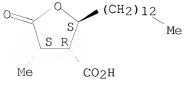
II



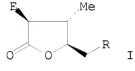
III

AB (-)-Dihydroprotolichesterinic acid I is synthesized in 6 steps and 57% overall yield by a strategy employing the camphene-derived chiral auxiliary II to construct the three contiguous stereogenic centers in consecutive stereocontrolled 1,4-conjugate addition of crotonyl imide III and syn-aldol reaction of tetradecanal with the vinylmagnesium bromide adduct of III.
IT 144356-39-8P, (-)-Dihydroprotolichesterinic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dihydroprotolichesterinic acid via stereocontrolled conjugate addition and syn-aldol)
RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



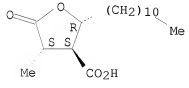
L14 ANSWER 50 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1994:557410 CAPLUS
DOCUMENT NUMBER: 121:157410
ORIGINAL REFERENCE NO.: 121:28493a,28496a
TITLE: New entry to chiral butenolide synthons. Application to expeditious syntheses of (+)-nephrosteranic acid, (+)-trans-whisky lactone, and (+)-trans-cognac lactone
AUTHOR(S): Takahata, Hiroki; Uchida, Yasuhiro; Momose, Takefumi
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharmaceut. Univ., Toyama, 930-01, Japan
SOURCE: Tetrahedron Letters (1994), 35(24), 4123-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:157410
GI



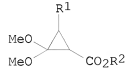
I

AB A new entry to chiral butenolide synthons starting with iodolactonization of the readily available, homochiral N-benzyl-N-methyl-3-hydroxy-4-pentenamide and its application to the syntheses of (+)-nephrosteranic acid I (R = C10H21, Nu, = CO2H, E = Me), (+)-trans-whisky lactone I (R = C3H7, Nu = Me, E = H), and (+)-trans-cognac lactone I (R = C4H9, Nu = Me, E = H) are described.
IT 70579-56-5P, (+)-Nephrosteranic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of)
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(CA INDEX NAME)

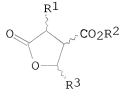
Absolute stereochemistry.



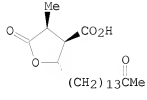
L14 ANSWER 51 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:603247 CAPLUS
DOCUMENT NUMBER: 119:203247
ORIGINAL REFERENCE NO.: 119:36241a,36244a
TITLE: Ring-opening aldol-type reaction of 2,2-dialkoxycyclopropanecarboxylic esters with carbonyl compounds. 3. The diastereoselective synthesis of 2,3,4-trisubstituted γ-lactones
AUTHOR(S): Shimada, Shigeru; Hashimoto, Yukihiko; Saigo, Kazuhiko
CORPORATE SOURCE: Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Journal of Organic Chemistry (1993), 58(19), 5226-34
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203247
GI



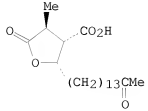
I



II



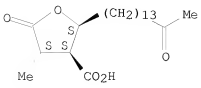
III



IV

AB The Lewis acid-promoted reaction of 3-alkyl-2,2-dialkoxycyclopropanecarboxylic esters I (R1 = R2 = Me, Et; R1 = Me, R2 = Et, CMe3; R1 = CHMe2, R2 = Et) with R3CHO (R3 = cyclohexyl, n-heptyl, CHMe2, CMe3, Ph, PhCH2CH2) to give 2,3,4-trisubstituted γ-lactones II (trans-trans, trans-cis, cis-trans, cis-cis) was investigated. The diastereoselectivity of this reaction is highly dependent on the catalyst employed. Thus while the ZrCl4-promoted reaction gave (2α,3α,4β)-trisubstituted γ-lactones in good yields with excellent selectivity, the SnBr4-promoted reaction was moderately selective for (2α,3α,4α)-trisubstituted γ-lactones. The present reaction was applied to the synthesis of (+)589- and (-)589-dihydropertusaric acid (III). Comparison of the spectroscopic and phys. data of synthetic III with those of a 4-alkyl-3-carboxy-2-Me γ-lactone isolated from the lichen Pertusaria albescens revealed that the relative stereochem. of the natural γ-lactone was not (2β,3β,4α), as reported by Huneck and his co-workers, but rather (2β,3α,4α); i.e., the natural γ-lactone was not (-)589-dihydropertusaric acid III, but (-)589-pertusarinic acid (IV).
IT 101899-68-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 101899-68-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



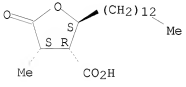
L14 ANSWER 52 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:495208 CAPLUS
DOCUMENT NUMBER: 119:95208
ORIGINAL REFERENCE NO.: 119:17157a,17160a
TITLE: First asymmetric synthesis of (+)- and (-)-roccellaric acid and dihydroprotolichesterinic acid
AUTHOR(S): Mulzer, Johann; Salimi, Nabiollah; Hartl, Hans
CORPORATE SOURCE: Inst. Org. Chem., Freie. Univ. Berlin, Berlin, W-1000/33, Germany
SOURCE: Tetrahedron: Asymmetry (1993), 4(3), 457-71
CODEN: TASYE3; ISSN: 0957-4166
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Stereocontrolled syntheses of the title compds. from (R)-2,3-isopropylideneglyceraldehyde, (S)-O-tetrahydropyranyllactaldehyde and 1,2:5,6-di-O-isopropylidene-α-D-glucofuranose (diacetone-D-glucose) are described.

IT 144356-39-8P 148676-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

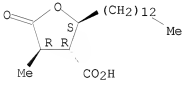
RN 144356-39-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 148676-05-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3R,4R)- (CA INDEX NAME)

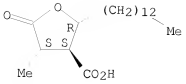
Absolute stereochemistry. Rotation (-).



IT 19464-85-8P 19464-87-0P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of)

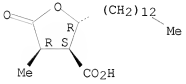
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

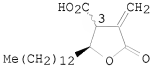


RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 53 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:630101 CAPLUS
DOCUMENT NUMBER: 117:230101
ORIGINAL REFERENCE NO.: 117:39701a,39704a
TITLE: Contribution to the chemistry of proto- and allo-protolichesterinic acids
AUTHOR(S): Huneck, Siegfried; Takeda, Reiji
CORPORATE SOURCE: Inst. Pflanzenbiochem., Halle/Saale, D-O-4050, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1992), 47(6), 842-54
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

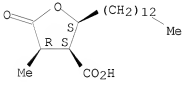


I, 3?
II, 3?

AB The isolation and spectroscopic characterization of (-)-allo-protoichesterinic acid (I) from Cetraria komarovii is described. Protolichesterinic acid (II) and I were transformed into numerous nitrogen-containing derivs. and the isomerization of the dihydro acids was investigated.

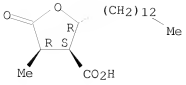
IT 493-45-8
RL: BIOL (Biological study)
(of Cetraria komarovii)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



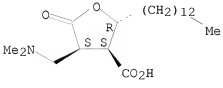
IT 19464-87-0P 144032-08-6P 144071-12-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



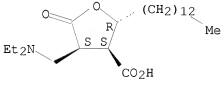
RN 144032-08-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[(dimethylamino)methyl]tetrahydro-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



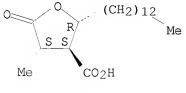
RN 144071-12-5 CAPLUS
CN 3-Furancarboxylic acid, 4-[(diethylamino)methyl]tetrahydro-5-oxo-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



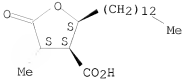
IT 19464-85-8P 133695-37-1P 144031-98-1P
144031-99-2P 144032-09-7P 144071-13-6P
144356-39-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

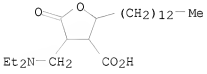


RN 133695-37-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

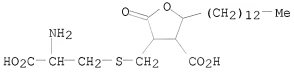
Absolute stereochemistry.



RN 144031-98-1 CAPLUS
CN 3-Furancarboxylic acid, 4-[(diethylamino)methyl]tetrahydro-5-oxo-2-tridecyl- (CA INDEX NAME)

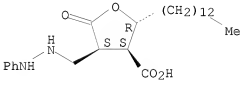


RN 144031-99-2 CAPLUS
CN 3-Furancarboxylic acid, 4-[[(2-amino-2-carboxyethyl)thio]methyl]tetrahydro-5-oxo-2-tridecyl- (CA INDEX NAME)



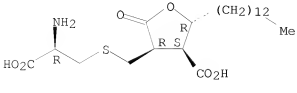
RN 144032-09-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-5-oxo-4-[(2-phenylhydrazino)methyl]-2-tridecyl-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 144071-13-6 CAPLUS
CN 3-Furancarboxylic acid, 4-[[(2-amino-2-carboxyethyl)thio]methyl]tetrahydro-5-oxo-2-tridecyl-, [2R-[2α,3β,4β(R*)]]- (9CI) (CA INDEX NAME)

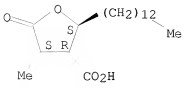
Absolute stereochemistry.



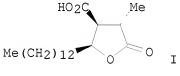
RN 144356-39-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 54 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:247032 CAPLUS
DOCUMENT NUMBER: 114:247032
ORIGINAL REFERENCE NO.: 114:41697a,41700a
TITLE: Highly Felkin-Anh selective Hiyama additions of chiral allylic bromides to aldehydes. Application to the first synthesis of nephromopsinic acid and its enantiomer
AUTHOR(S): Mulzer, Johann; Kattner, Lars; Strecker, Achim R.; Schroeder, Christian; Buschmann, Juergen; Lehmann, Christian; Luger, Peter
CORPORATE SOURCE: Inst. Org. Chem., Freie Univ. Berlin, Berlin, D-1000/33, Germany
SOURCE: Journal of the American Chemical Society (1991), 113(11), 4218-29
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:247032
GI



I

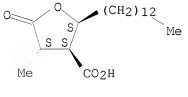
AB The Cr(II)-mediated addition (Hiyama reaction) of chiral allylic bromides to achiral and chiral aldehydes proceeds with high Felkin-Anh selectivity with respect to the stereocenter at C-γ in the bromide. Double stereodifferentiation expts. show that the bromide is the stereodominating component in the addition The methodol. was applied to the first synthesis of nephromopsinic acid (I), found in the lichen species Nephromopsis stracheyi, and its enantiomer. Crystal structures are reported for two of the adducts.

IT 133695-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
((-)-Nephromopsinic acid; total synthesis of)

RN 133695-37-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, [2S-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

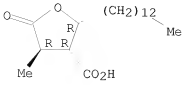


IT 133695-45-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of)

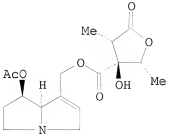
RN 133695-45-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 55 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:459636 CAPLUS
DOCUMENT NUMBER: 113:59636
ORIGINAL REFERENCE NO.: 113:10103a,10106a
TITLE: The absolute configurations of longitubine (7-O-acetyl-9-O-latifolylretronecine) and latifolic acid
AUTHOR(S): Stermitz, Frank R.; Hope, Hakon
CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins, CO, 80523, USA
SOURCE: Tetrahedron Letters (1989), 30(51), 7153-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

II

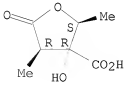
AB A single crystal x-ray study established the absolute configuration of longitubine (7-O-acetyl-9-O-latifolylretronecine) (I) and hence that of latifolic acid (II). The absolute configuration of latifolic acid conforms with that established chemical by Matsumoto, Okabe and Fukui, and consequently is not in agreement with that purportedly established through an x-ray study by Roitman and Wong.

IT 50460-79-2, (+)-Latifolic acid
RL: PRP (Properties)
(absolute configuration of)

RN 50460-79-2 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



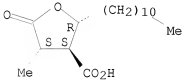
L14 ANSWER 56 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:88475 CAPLUS
DOCUMENT NUMBER: 112:88475
ORIGINAL REFERENCE NO.: 112:14879a,14882a
TITLE: Nonsymmetric spherulites: nephrasteranic acid
AUTHOR(S): Prasad, P. B. V.; Prasad, N. Durga
CORPORATE SOURCE: Dep. Phys., Gov. Polytech., Warangal, 506007, India
SOURCE: Crystal Research and Technology (1989), 24(10), K183-K186
CODEN: CRTEDF; ISSN: 0232-1300
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sym. and asym. spherulitic crystallization of nephrasteranic acid is discussed. The extent of asymmetry observed in the present case is employed to make certain qual. estns.

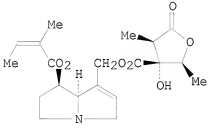
IT 70579-56-5, Nephrasteranic acid
RL: PRP (Properties)
(crystallization of nonsym. spherulites of)

RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-
(CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 57 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:595198 CAPLUS
DOCUMENT NUMBER: 111:195198
ORIGINAL REFERENCE NO.: 111:32459a,32462a
TITLE: Revised absolute configurations of latifolic acid and the pyrrolizidine alkaloid latifoline
AUTHOR(S): Roitman, James N.; Wong, Rosalind Y.
CORPORATE SOURCE: West. Reg. Res. Cent., Agric. Res. Serv., Albany, CA, 94710, USA
SOURCE: Australian Journal of Chemistry (1988), 41(11), 1781-7
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

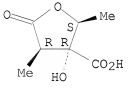
AB The absolute stereochem. of (+)-latifolic acid has been determined by single-crystal x-ray crystallog. anal. to be (2S,3R,4R)-3-hydroxy-2,4-dimethyl-5-oxotetrahydrofuran-3-carboxylic acid. The configuration of the three chiral centers is opposite to that presently recorded in the literature. Accordingly, the configuration of the pyrrolizidine alkaloid, latifoline (I) which includes a latifolic acid side chain, must be revised.

IT 50460-79-2, Latifolic acid
RL: PRP (Properties)
(crystal structure and absolute configuration of)

RN 50460-79-2 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



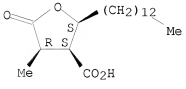
L14 ANSWER 58 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:489797 CAPLUS
DOCUMENT NUMBER: 109:89797
ORIGINAL REFERENCE NO.: 109:14927a,14930a
TITLE: Lichen constituents. Part 149: Components of some lichens from Mongolia
AUTHOR(S): Huneck, S.; Tuja, D.; Cogt, U.
CORPORATE SOURCE: Inst. Biochem., Akad. Wiss. DDR, Halle/Saale, Ger. Dem. Rep.
SOURCE: Pharmazie (1988), 43(5), 371-2
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Aspicilia vagans From the Mongolian Altai contained triglycerides and phytosterols. Cetraria tilesii Contained pinastric, (-)-usnic, and vulpinic acids, Dactylina madreporiformis contained (+)-usnic and (-)-nephromopsic acids, Rhizoplaca baranowii contained (-)-usnic and psoromic acids, triglycerides, and phytosterols, and Xanthoria elegans contained parietin.

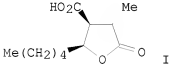
IT 493-45-8
RL: BIOL (Biological study)
(in lichens from Mongolian Altai)

RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



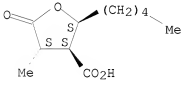
L14 ANSWER 59 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:473910 CAPLUS
DOCUMENT NUMBER: 107:73910
ORIGINAL REFERENCE NO.: 107:12117a,12120a
TITLE: Structure and stereochemistry of phaseolinic acid: a new acid from Macrophomina phaseolina
AUTHOR(S): Mahato, Shashi B.; Siddiqui, Kazi A. I.; Bhattacharya, Gautam; Ghosal, Tapasree; Miyahara, Kazumoto; Sholichin, Mochammad; Kawasaki, Toshio
CORPORATE SOURCE: Indian Inst. Chem. Biol., Calcutta, 700 032, India
SOURCE: Journal of Natural Products (1987), 50(2), 245-7
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



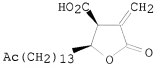
I

AB A new acid designated phaseolinic acid (I) was isolated from the culture filtrate of M. phaseolina. The structure of I was determined by its IR, 1H NMR, and mass spectra and single crystal x-ray crystallog. The absolute configuration of I was 2R,3R,4R.
IT 109667-12-1
RL: BIOL (Biological study)
(from Macrophomina phaseolina, isolation and structure determination of)
RN 109667-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2S,3S,4S)- (CA INDEX NAME)

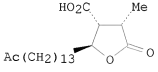
Absolute stereochemistry. Rotation (-).



L14 ANSWER 60 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1986:183270 CAPLUS
DOCUMENT NUMBER: 104:183270
ORIGINAL REFERENCE NO.: 104:28969a,28972a
TITLE: Lichen substances. Part 144. (-)-Allo-pertusaric acid and (-)-dihydropertusaric acid from the lichen Pertusaria albescens
AUTHOR(S): Huneck, Siegfried; Toensberg, Tor; Bohlmann, Ferdinand
CORPORATE SOURCE: Inst. Plant Biochem., Ger. Acad. Sci., Halle/Saale, 4010, Ger. Dem. Rep.
SOURCE: Phytochemistry (Elsevier) (1986), 25(2), 453-9
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



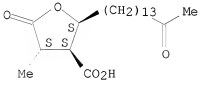
I



II

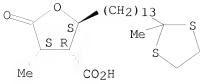
AB The structures of 2 γ-lactone carboxylic acids from the lichen P. albescens, (-)-allo-pertusaric acid (I) and (-)-dihydropertusaric acid (II), were elucidated by spectroscopic and chemical methods. From P. ophthalmiza, taraxerone and a mixture of long-chain aliphatic alcs. and fatty acids were isolated.
IT 101899-68-7
RL: BIOL (Biological study)
(of Pertusaria albescens, structure of)
RN 101899-68-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2S,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



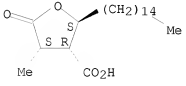
IT 101899-75-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation and desulfurization of)
RN 101899-75-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-[13-(2-methyl-1,3-dithiolan-2-yl)tridecyl]-5-oxo-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



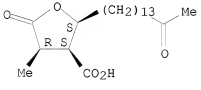
IT 101899-66-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 101899-66-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentadecyl-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



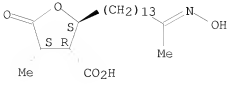
IT 101899-63-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with diazomethane)
RN 101899-63-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, [2S-(2α,3α,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 101899-69-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 101899-69-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[14-(hydroxyimino)pentadecyl]-4-methyl-5-oxo-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



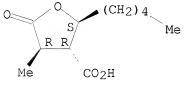
L14 ANSWER 61 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:592767 CAPLUS
DOCUMENT NUMBER: 103:192767
ORIGINAL REFERENCE NO.: 103:30981a,30984a
TITLE: Metabolites of the higher fungi. Part 2. 2-Butyl-3-methylsuccinic acid and 2-hexylidene-3-methylsuccinic acid from xylariaceous fungi
AUTHOR(S): Anderson, John R.; Edwards, Raymond L.; Whalley, Anthony J. S.
CORPORATE SOURCE: Sch. Chem., Univ. Bradford, Bradford, BD7 1DP, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (7), 1481-5
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The diacid (+)-erythro-HO2CCHMeCHBuCO2H was isolated from Hypoxylon illitum. (+)-(E)-HO2CCHMeC(CO2H):CH(CH2)4Me [(+)-(E)-I] was isolated from H. deustum, (-)-(E)-I from Xylaria polymorpha, X. longipes, and Poronia piliformis, and the racemic (E)-I was obtained from X. mali and X. hypoxylon. The structures and configurations of these compds. were determined by spectral and synthetic methods.

IT 98985-82-1P 98985-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

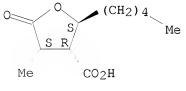
RN 98985-82-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3S,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.



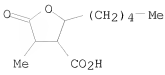
RN 98985-83-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl-, (2R,3S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



IT 98985-77-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 98985-77-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-pentyl- (CA INDEX NAME)


O
O
(CH2)4—Me
Me
CO2H

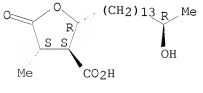
L14 ANSWER 62 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:607615 CAPLUS
DOCUMENT NUMBER: 101:207615
ORIGINAL REFERENCE NO.: 101:31403a,31406a
TITLE: Ecological and chemical investigations of lichens from South Georgia and the maritime Antarctic
AUTHOR(S): Huneck, S.; Sainsbury, M.; Rickard, T. M. A.; Smith, R. I. Lewis
CORPORATE SOURCE: Inst. Plant Biochem., Acad. Sci. GDR, Halle/Saale, GDR-401, Ger. Dem. Rep.
SOURCE: Journal of the Hattori Botanical Laboratory (1984), 56, 461-80
CODEN: JHBLAI; ISSN: 0073-0912
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Compds. of a possible chemotaxonomic importance found in 20 lichen taxa, which were collected in 5 localities of South Georgia and in the maritime Antarctic, are described. Parietin, fumarprotocetraric acid, atranorin, arthothelin, barbatolic acid , zeorin,, protocetraric acid,, calycin, 2α-acetoxystictane-3β,22α-diol, stictane-2α,3β,22α-triol, pseudocyphellarin A and B, (-)-usnic acid, stictic acid, constictic acid, 7β-acetoxyhopane-22-ol, hopane-15α,22-diol, (+)-usnic acid, rhizocarpic acid, psoromic acid, thamnolic acid, sphaerophorin, lobaric acid, , murolic acid, neodihydromurolic acid, and salazinic acids were found in Caloplaca regalis, Cladonia gracilis, C. pycnoclada, C. rangiferina, Haematomma erythromma, Himantormia lugubris, Lecidella bullata, Pertusaria dactylina, Pseudocyphellaria endochrysa, P. freycinetti, Ramalina terebrata, Rhizocarpon geographicum, Sphaerophorus globosus, Stereocaulon glabrum, Usnea antarctica, U. fasciata, and U. sulphurea, in a chemotaxonomically characteristic manner. In Umbilicaria antarctica, gyrophoric acid, a mixture of sterols, trilinolein and other triglycerides with oleic, palmitic, and palmitoleic acids were found. U. decussata Contained a mixture of triglycerides almost identical with that in U. antarctica. In Leptogium menziesii, 14 compds., none of which could be identified, were found in the ether exts. The ecol. of each taxon is given.

IT 70579-57-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of lichens from South Georgia and maritime Antarctic)

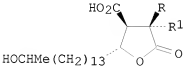
RN 70579-57-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.

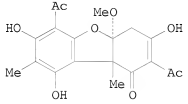


L14 ANSWER 63 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:607428 CAPLUS
DOCUMENT NUMBER: 91:207428
ORIGINAL REFERENCE NO.: 91:33387a,33390a
TITLE: Recent results in the chemistry of lichen substances
AUTHOR(S): Huneck, Siegfried
CORPORATE SOURCE: Inst. Plant Biochem., Ger. Acad. Sci., Halle/Saale, DDR-401, Ger. Dem. Rep.
SOURCE: Symp. Pap. - IUPAC Int. Symp. Chem. Nat. Prod., 11th (1978), Volume 4, Issue Part 1, 197-206. Editor(s): Marekov, N.; Ognyanov, I.; Orahovats, A. Izd. BAN: Sofia, Bulg.
CODEN: 41RTAX
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



I, RR1=CH2
II, R=H, R1=Me



III

AB In studies on lichen substances, the structures of 2 γ-lactone carboxylic acids, 2 δ-lactone carboxylic acids, 3 chloroxanthones, and a new dibenzofuran derivative were elucidated. Lecanora muralis Yielded murolic (I) and neodihydromurolic (II) acids, along with (+)-usnic acid, psoromic acid, zeorin, and leucotylin. I and II were also found in L. melanophthalma and L. rubins. The latter species also contained (-)-pseudoplacodiolic acid (III). Pertusaria aleianta Contained a mixture of chloroxanthones: 2,5-dichlorolichexanthone, 2,4-dichlorolichexanthone, and 2,4,5-trichlorolichexanthone. Acarospora chlorophane Contained acaranoic and acarenoic acids.

IT 70579-57-6
RL: BIOL (Biological study)
(from Lecanora species)

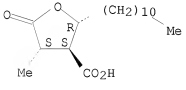
RN 70579-57-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.

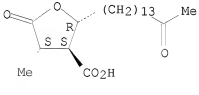
L14 ANSWER 64 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:435683 CAPLUS
DOCUMENT NUMBER: 91:35683
ORIGINAL REFERENCE NO.: 91:5803a,5806a
TITLE: Neodihydromurol and murolic acid, two new γ-lactonecarboxylic acids from Lecanora muralis
AUTHOR(S): Huneck, Siegfried; Schreiber, Klaus; Hoefle, Gerhard; Snatzke, Guenther
CORPORATE SOURCE: Inst. Biochem., DAW, Halle/Saale, DDR-401, Ger. Dem. Rep.
SOURCE: Journal of the Hattori Botanical Laboratory (1979), 45, 1-23
CODEN: JHBLAI; ISSN: 0073-0912
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Two new aliphatic hydroxy γ-lactone carboxylic acids, (+)-neodihydromurolic acid and (+)-murolic acid, were isolated from the lichens Lecanora muralis, L. melanophthalma, and L. rubina. Spectroscopical and chemical data led to the following structures: (+)-neodihydromurolic acid, (+)-2(S)-methy-3(S)-carboxy-4(R),18(R)-dihydroxynonadecan-1→4-olide (I); and (+)-murolic acid, (+)-2-methylen-3(S)-carboxy-4(R),18(R)-dihydroxynonadecan-1→4-olide (II). The absolute configurations of (+)-nephrosteranic acid, (-)-alloprotolichesterinic acid, and (+)-nephrosterinic acid were established.
IT 70579-56-5P 70579-60-1P 70579-70-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 70579-56-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2R,3S,4S)-(CA INDEX NAME)

Absolute stereochemistry.



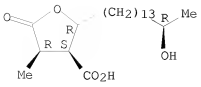
RN 70579-60-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(14-oxopentadecyl)-, (2R,3S,4S)- (CA INDEX NAME)

Absolute stereochemistry.



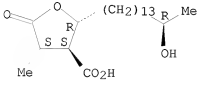
RN 70579-70-3 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 70579-57-6
RL: BIOL (Biological study)
(Lecanora lactonecarboxylic acid)
RN 70579-57-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[(14R)-14-hydroxypentadecyl]-4-methyl-5-oxo-, (2R,3S,4S)- (CA INDEX NAME)

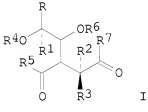
Absolute stereochemistry.



L14 ANSWER 65 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:38683 CAPLUS
DOCUMENT NUMBER: 90:38683
ORIGINAL REFERENCE NO.: 90:6223a,6226a
TITLE: Phenylpentanoic acid derivatives
INVENTOR(S): Aldridge, David Cecil; Crawley, Graham Charles; Strawson, Colin John
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd., UK
SOURCE: Ger. Offen., 37 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2804083	A1	19780824	DE 1978-2804083	19780131
ZA 7800437	A	19781227	ZA 1978-437	19780124
NL 7801435	A	19780818	NL 1978-1435	19780208
BE 863995	A1	19780816	BE 1978-185202	19780215
SE 7801756	A	19780816	SE 1978-1756	19780215
FI 7800488	A	19780817	FI 1978-488	19780215
FR 2381040	A1	19780915	FR 1978-4284	19780215
DK 7800702	A	19780817	DK 1978-702	19780216
JP 53103443	A	19780908	JP 1978-17089	19780216

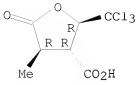
PRIORITY APPLN. INFO.: GB 1977-6450 A 19770216
OTHER SOURCE(S): MARPAT 90:38683
GI



I

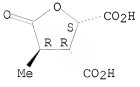
AB Phenylpentanoic acids I (R or R1 = Ph, optionally substituted with halo, NO2, NH2, alkyl, alkoxy or alkanoyl, the other R or R1 = H; R2 or R3 = H or C1-4 alkyl, the other R2 or R3 = H; R4 = H, R5 = OH, or R4R5 = a direct bond; R6 = H, R7 = OH, or R6R7 = a direct bond), useful for the treatment of duodenal ulcers (no data) were prepared Thus, nitration of I (R = Ph, R1 = R2 = H, R3 = Me, R4R5 and R6R7 = direct bonds) in concentrated HNO3 gave I (R = 4-O2NC6H4, R1-R7 unchanged) (II) and 2 position isomers, and II treated with H in AcOH-Ac2O gave I (R = 4-AcNHC6H4, R1-R7 unchanged).
IT 68836-30-6P 68836-31-7P 68836-36-2P
68836-38-4P 68836-39-5P 68836-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 68836-30-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-(trichloromethyl)-, (2R,3R,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



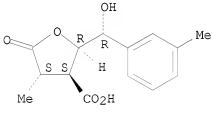
RN 68836-31-7 CAPLUS
CN Xylaric acid, 3-carboxy-2,3-dideoxy-2-methyl-, 1,4-lactone (9CI) (CA INDEX NAME)

Relative stereochemistry.



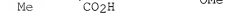
RN 68836-36-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[hydroxy(3-methylphenyl)methyl]-4-methyl-5-oxo-, [2α(R*),3α,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



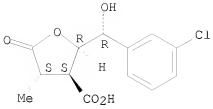
RN 68836-38-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[hydroxy(4-methoxyphenyl)methyl]-4-methyl-5-oxo-, [2α(R*),3α,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



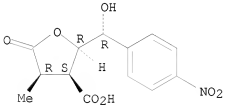
RN 68836-39-5 CAPLUS
CN 3-Furancarboxylic acid, 2-[(3-chlorophenyl)hydroxymethyl]tetrahydro-4-methyl-5-oxo-, [2α(R*),3α,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 68836-40-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-[hydroxy(4-nitrophenyl)methyl]-4-methyl-5-oxo-, [2α(R*),3α,4α]- (9CI) (CA INDEX NAME)

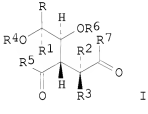
Relative stereochemistry.



L14 ANSWER 66 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:38540 CAPLUS
DOCUMENT NUMBER: 90:38540
ORIGINAL REFERENCE NO.: 90:6199a,6202a
TITLE: Hydroxy acids
INVENTOR(S): Adlridge, David Cecil; Crawley, Graham Charles; Strawson, Colin John
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd., UK
SOURCE: Ger. Offen., 57 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2804084	A1	19780817	DE 1978-2804084	19780131
ZA 7800438	A	19781227	ZA 1978-438	19780124
NL 7801434	A	19780818	NL 1978-1434	19780208
BE 863994	A1	19780816	BE 1978-185201	19780215
SE 7801755	A	19780816	SE 1978-1755	19780215
FI 7800487	A	19780817	FI 1978-487	19780215
FR 2381041	A1	19780915	FR 1978-4288	19780215
DK 7800701	A	19780817	DK 1978-701	19780216
JP 53103467	A	19780908	JP 1978-17088	19780216
PRIORITY APPLN. INFO.:			GB 1977-6448 A	19770216
			GB 1977-6449 A	19770216
			GB 1977-19772 A	19770511

OTHER SOURCE(S): MARPAT 90:38540
GI



I

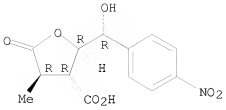
AB Dihydroxydicarboxylic acid monolactones I (one of R and R1 is H, C1-6 alkyl, or substituted-phenyl and the other is H; one of R2 and R3 is H or C1-4 alkyl and the other is H; R4 = H, R5 = OH, and R6R7 = direct bond, or R4R5 = direct bond, R6 = H, and R7 = OH) and their esters, useful as inhibitors of gastric juice secretion (no data), were prepared Thus, cis-3α-carboxy-2β-methyl-4-nonenoic acid stirred 1 h at 40° with H2O2 in HCO2H gave 47% I (R = Bu, R1 = R2 = R4 = H, R3 = Me, R5 = OH, R6R7 = direct bond).

IT 68657-74-9P 68657-75-0P 68657-76-1P
68686-64-6P 68686-65-7P 68686-66-8P
68686-71-5P 68686-72-6P 68845-61-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68657-74-9 CAPLUS

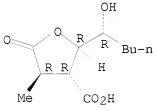
CN 3-Furancarboxylic acid, tetrahydro-2-[hydroxy(4-nitrophenyl)methyl]-4-methyl-5-oxo-, [2α(R*),3β,4α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



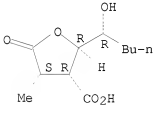
RN 68657-75-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3β,4α]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



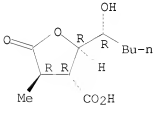
RN 68657-76-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3β,4β]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



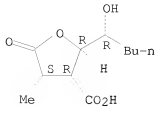
RN 68686-64-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3β,4α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



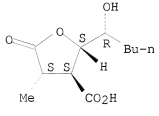
RN 68686-65-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3β,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



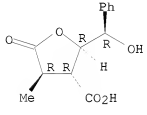
RN 68686-66-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(S*),3β,4α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



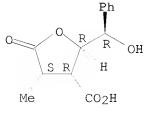
RN 68686-71-5 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(hydroxyphenylmethyl)-4-methyl-5-oxo-, [2α(R*),3β,4α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 68686-72-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(hydroxyphenylmethyl)-4-methyl-5-oxo-, [2α(R*),3β,4β]- (9CI) (CA INDEX NAME)

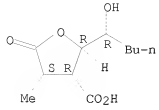
Relative stereochemistry.



RN 68845-61-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-,

monosodium salt, [2α(R*),3β,4β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

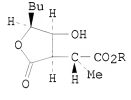


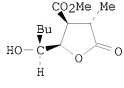
● Na

L14 ANSWER 67 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:502100 CAPLUS
DOCUMENT NUMBER: 87:102100
ORIGINAL REFERENCE NO.: 87:16199a,16202a
TITLE: Esters of hydroxy alkanoic acids
AUTHOR(S): Anon.
CORPORATE SOURCE: UK
SOURCE: Research Disclosure (1977), 158, 81-2 (No. 15848)
CODEN: RSDSBB; ISSN: 0374-4353
DOCUMENT TYPE: Journal; Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RD 158048		19770610	RD 1977-158048	19770610

PRIORITY APPLN. INFO.: RD 1977-158048 19770610
GI


I


II

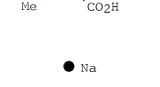
AB The hydroxy esters I (R = Me, benzyl, Et, phenacyl), with useful ulcer-healing properties, were prepared in 68-90% yield by treating I (R = H) Na salt with the corresponding halide. Me 2α-methyl-3β-carboxy-4β,5β-dihydroxynonanoate was also prepared II was prepared similarly in 70% yield from the resp. acid.

IT 63776-55-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)

RN 63776-55-6 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, monosodium salt, [2α(R*),3α,4β]-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

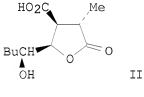


● Na

L14 ANSWER 68 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:438888 CAPLUS
DOCUMENT NUMBER: 87:38888
ORIGINAL REFERENCE NO.: 87:6123a,6126a
TITLE: Hydroxy acids
INVENTOR(S): Aldridge, David Cecil; Crawley, Graham Charles; Strawson, Colin John
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd., UK
SOURCE: Ger. Offen., 42 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2637597	A1	19770303	DE 1976-2637597	19760820
GB 1538440	A	19790117	GB 1975-34842	19760723
IN 143354	A1	19771105	IN 1976-CA1357	19760729
AU 502751	B2	19790809	AU 1976-16415	19760730
DK 7603721	A	19770222	DK 1976-3721	19760818
FI 7602352	A	19770222	FI 1976-2352	19760818
SU 667126	A3	19790605	SU 1976-2387220	19760818
SE 7609234	A	19770222	SE 1976-9234	19760819
BE 845403	A1	19770221	BE 1976-169984	19760820
NO 7602873	A	19770222	NO 1976-2873	19760820
NL 7609266	A	19770223	NL 1976-9266	19760820
JP 52025718	A	19770225	JP 1976-99566	19760820
FR 2321278	A1	19770318	FR 1976-25396	19760820
FR 2321278	B1	19781117		
DD 125833	A5	19770518	DD 1976-194419	19760820
CH 622765	A5	19810430	CH 1976-10617	19760820
US 4145437	A	19790320	US 1977-845420	19771025
PRIORITY APPLN. INFO.:			GB 1975-34842 A	19750821
			US 1976-716284 A1	19760820

OTHER SOURCE(S): MARPAT 87:38888
GI



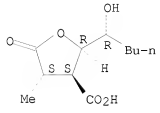
II

AB Antiinflammatory (no data) optically-active hydroxy acids RCOCH[CH(OR1)CR2R3OR4]CR5R6COR7 (I; R and R7 = OH, R1 and R4 = H, or RR7 and/or R1R4 = a direct bond; R2, R3 = independently H, alkyl, or Ph; R5, R6 = independently H or alkyl) were prepared by hydrolysis of a lactone or dilactone, or by removal of a protective group from a protected hydroxy acid. Among I thus prepared were (R-R7 given): R = OH, R1R7 = direct bond, R2 = R4 = R5 = H, R3 = Bu, R6 = Me (II); and R = R7 = OH, R1 = R4 = R6 = H, R2 = Bu, R5 = Me.

IT 63126-55-6P 63126-58-9P 63126-61-4P
63126-64-7P
RL: SPN (Synthetic preparation); PREP (Preparation)

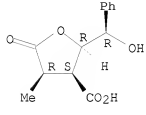
(preparation of)
RN 63126-55-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3α,4β]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



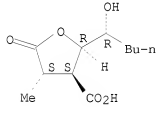
RN 63126-58-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(hydroxyphenylmethyl)-4-methyl-5-oxo-, [2α(R*),3α,4α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 63126-61-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, monosodium salt, [2α(R*),3α,4β]-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.



● Na

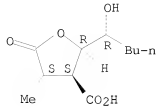
RN 63126-64-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2-(1-hydroxypentyl)-4-methyl-5-oxo-, [2α(R*),3α,4β]-(-)-, compd. with N-ethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 63126-55-6

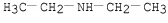
CMF C11 H18 O5

Rotation (-). Absolute stereochemistry unknown.



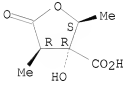
CM 2

CRN 109-89-7
CMF C4 H11 N



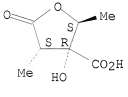
L14 ANSWER 69 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:505447 CAPLUS
DOCUMENT NUMBER: 79:105447
ORIGINAL REFERENCE NO.: 79:17103a,17106a
TITLE: Pyrrolizidine alkaloids. Absolute configurations of latifolic acid and its stereoisomers
AUTHOR(S): Matsumoto, Takashi; Okabe, Tetsuaki; Fukui, Kenji
CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, Japan
SOURCE: Chemistry Letters (1973), (8), 773-6
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Latifolic acid (I) from Cynoglossum latifolium has the absolute configuration (3R,4S,5S), based on its synthesis from (±)-4-hydroxy-3-(methoxycarbonyl)-2,4-dimethylbutyrolactone. Thus, latifoline (II) has the same absolute configuration.
IT 50460-79-2
RL: PRP (Properties)
(absolute configuration of)
RN 50460-79-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



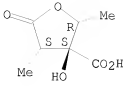
IT 50460-92-9P 50460-94-1P 50460-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50460-92-9 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



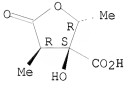
RN 50460-94-1 CAPLUS
CN L-threo-Pentonic acid, 3-C-carboxy-2,5-dideoxy-2-C-methyl-, γ-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



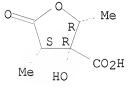
RN 50460-97-4 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



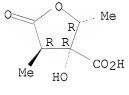
L14 ANSWER 70 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:99166 CAPLUS
DOCUMENT NUMBER: 76:99166
ORIGINAL REFERENCE NO.: 76:15951a,15954a
TITLE: Senecio alkaloids. Synthesis and configuration of (+-)-latifolic acid
AUTHOR(S): Matsumoto, Takashi; Okabe, Tetsuaki; Fukui, Kenji
CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, Japan
SOURCE: Chemistry Letters (1972), (1), 29-32
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB ±)-Latifolic acid (I) (identical (ir) with the (±)-isomer of natural latifolic acid) and its 3 stereoisomeric racemates were prepared from di-Me 1-acetyl-2-methylsuccinate.
IT 35493-70-0P 35493-72-2P 35493-76-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35493-70-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, (2α,3α,4α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



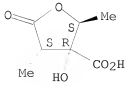
RN 35493-72-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, (2α,3α,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 35493-76-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, (2α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



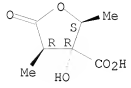
IT 35493-74-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from dimethyl acetyl methylsuccinate, configuration of)

RN 35493-74-4 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, (2α,3β,4α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

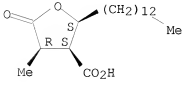


L14 ANSWER 71 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:77124 CAPLUS
DOCUMENT NUMBER: 70:77124
ORIGINAL REFERENCE NO.: 70:14369a,14372a
TITLE: Naturally occurring lactones and lactams. I. Absolute configuration of ranunculin, lichesterinic acid, and some lactones related to lichesterinic acid
AUTHOR(S): Boll, Per M.
CORPORATE SOURCE: Univ. Copenhagen, Copenhagen, Den.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1968), 22(10), 3245-50
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N.M.R. spectra have confirmed the provisional structure of ranunculin. Circular dichroism data allowed the assignment of the configuration of its aglucone to be 4S. As a result of the circular dichroism work, it was also possible to allocate configurations to the following lichen lactones: (S)-(-)-lichesterinic acid, (3R,4S)-(-)-protolichesterinic acid, (3S,4S)-(-)-alloprotolichesterinic acid, and (2R,3S,4S)-nephromopsic acid.

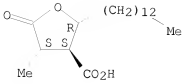
IT 493-45-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



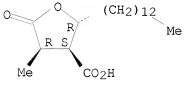
L14 ANSWER 72 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1968:49000 CAPLUS
DOCUMENT NUMBER: 68:49000
ORIGINAL REFERENCE NO.: 68:9455a,9458a
TITLE: Lichen constituents. XXXV. Chilean lichens. 14. Components of Rocellaria % mollis and the structure and absolute configuration of roccellaric acid
AUTHOR(S): Huneck, Siegfried; Follmann, Gerhard
CORPORATE SOURCE: Tech. Univ. Dresden, Tharandt, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (1967), 22(6), 666-70
CODEN: ZENBAX; ISSN: 0044-3174
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB R. mollis (77 g.) was extracted with Et2O 10 hrs., the extract shaken with aqueous NaHCO3 solution, which was acidified and again extracted with Et2O. The residue on evaporation of this last Et2O extract recrystd. from HOAc and then from MeOH yielded 1.75% roccellaric acid (I), m. 110-11°, [α]20D 35° (c 1.73, CHCl3); Me ester m. 40-1°, [α]20D 25° (c 1.53, CHCl3). Protolichesteric acid (II) was prepared by extracting Cetraria islandica with Et2O, extracting the ether extract with aqueous NaHCO3 acidifying, and extracting with Et2O; m. 107-8°, [α]20D 15° (c 4.73, CHCl3). II was converted into (+)-dihydroprotolichesteric acid (III) by hydrogenation with Pd-charcoal in HOAc, m. 104-6°; Me ester m. 50-1°, [α]20D 60° (c 1.76, CHCl3). III was reduced with 0.0428 g. Na in 9.6 ml. MeOH, 1 hr. on a steam bath, the mixture diluted with 20 ml. water, acidified with 10% H2SO4 and extracted with Et2O to give the Me ester (IV) of (+)-neo-dihydroprotolichesteric acid (V). Saponification of IV with NaOH in MeOH 5 days at room temperature gave V, m. 110-11°, [α]20D 38° (c 1.77, CHCl3). Comparison of V and IV were identical with I and its Me ester, resp. Reduction with LiAlH4 of the Me ester of I gave needles m. 59-61°, [α]20D 10° (c 1.29, CHCl3). The residue of R. mollis from the extraction with Et2O was extracted with acetone, the extracted residue extracted with water and the water extract evaporated Recrystn. from EtOH yielded 0.02% meso-erythritol, m. 119-20°. The residue from the extraction with water was dried and recrystd. from acetone, yielding 1.96% mollin, m. 270-1° (decomposition); acetyl derivative m. 208-9° (MeOH). The acetone mother liquor from the crystallization of mollin was concentrated and the residue recrystd. from HOAc to yield 1.3% roccellin, m. 206-7°, acetyl derivative m. 210°. Mollin and roccellin are new compds. Study of the O.R.D. curve of (+)-neo-dihydroprotolichesteric acid Me ester and its hydrogenation product and reference to the literature on similar compds., e.g. roccellic acid whose configuration was worked out by Akermark established the configuration I for roccellaric acid, 4-carboxy-3-methyl-2-oxo-5-tridecyltetrahydrofuran.
IT 19464-85-8P
RL: PREP (Preparation)
(from Roccellaria mollis)
RN 19464-85-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S,4S)-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 19464-87-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19464-87-0 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-,
[2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 73 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	1967:497597 CAPLUS
DOCUMENT NUMBER:	67:97597
ORIGINAL REFERENCE NO.:	67:18339a,18342a
TITLE:	Lichens. IV. Thin-layer chromatography of lichen substances
AUTHOR(S):	Santesson, Johan
CORPORATE SOURCE:	Univ. Uppsala, Uppsala, Swed.
SOURCE:	Acta Chemica Scandinavica (1947-1973) (1967), 21(5), 1162-72 CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE:	Journal
LANGUAGE:	English

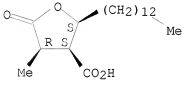
AB cf. CA 67: 51056p. The thin-layer chromatography on precoated plates of >80 lichen substances is described. 32 references.

IT 493-45-8
RL: ANT (Analyte); ANST (Analytical study)
(thin-layer chromatog. of)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



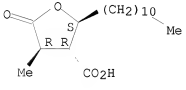
L14 ANSWER 74 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:475198 CAPLUS
DOCUMENT NUMBER: 65:75198
ORIGINAL REFERENCE NO.: 65:14079a-b
TITLE: Lichens. II. Thin-layer chromatography of aliphatic lichen acids
AUTHOR(S): Bendz, Gerd; Santesson, Johan; Tibell, Leif
CORPORATE SOURCE: Univ. Uppsala, Swed.
SOURCE: Acta Chemica Scandinavica (1966), 20(4), 1180-1
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 13073b. Aliphatic lichen acids were separated by thin layer chromatog. on silica gel HF, by using 40 mg. bromcresol green in 100 mL. 0.01N NaOH as the detection spray. Rf values were tabulated.Rf + 100 in solvent system, A, B, C, D; Caperatic acid, 03, 02, 01, 11; Lichesterinic acid, 73, 32, 56, X; Nephromopsinic acid, 82, 32, 54, X; Nephrosteranic acid, 82, 31, 55, X; Nephrosterinic acid, 61, 22, 43, X, Norrangiformic acid, 04, 03, 03, 49; Acaranoic acid, 68, 26, 42, X; Acarenoic acid, 48, 17, 30, X; Protolichesterinic acid, 61, 23, 43, X; Rangiformic acid, 50, 10, 36, 66; Roccellic acid, 91, 24, 60, X; X indicates that the acid travels with the secondary front; the solvents were: (A) ether-butyric acid 20:1, (B) CHCl3-propionic acid 20:1, (C) iso-Pr ether-propionic acid 20: 1, (D) CHCl3-HOAc 5:1.

IT 480-71-7, Nephrosteranic acid 493-45-8, Nephromopsinic acid
(chromatog. of)

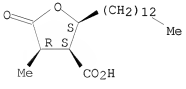
RN 480-71-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



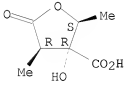
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.

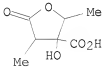


L14 ANSWER 75 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:15012 CAPLUS
DOCUMENT NUMBER: 58:15012
ORIGINAL REFERENCE NO.: 58:2478a-c
TITLE: Identity of the alkaloid from Crotalaria damarensis with (--)-1-methylenepyrrolizidine, now shown to occur partially racemized in C. anagroides H. B. and K.
AUTHOR(S): Culvenor, C. C. J.; Smith, L. W.
CORPORATE SOURCE: Commonwealth Sci. Ind. Res. Organ., Melbourne
SOURCE: Australian Journal of Chemistry (1962), 15, 328-31
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 53, 20107c. The liquid alkaloid from C. damarensis (Louw, CA 47, 12765i) occurs in the seeds as 1.35% free base and 0.45% N-oxide. It is 1-methylenepyrrolizidine (I), b150 115°, [α]18D -100° (c 0.86, alc.); picrate m. 218-19°, [α]18D -14.9° (c 0.94, Me2CO); tartrate (II) m. 98-100°, [α]D -0.7° (c 0.76, alc.); 3-bromocamphor-8-sulfonate (III) m. 179, [α]18D -49° (c 1.62, alc.). I isolated from C. anagyroides had [α]18D -58°, and crystallization of II did not give optically pure base (Kochetkov, et al., CA 55, 16512d). Crystallization from C6H6 gave optically pure III, while from alc.-Et2O it gave inefficient concentration of (+)-base salt. Rotations and consts. are recorded for samples of optically impure I and derivs.
IT 50460-79-2 92350-64-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 50460-79-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

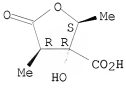


RN 92350-64-6 CAPLUS
CN Malic acid, 2-(1-hydroxyethyl)-3-methyl-, γ-lactone (7CI) (CA INDEX NAME)

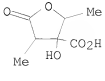


L14 ANSWER 76 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:15011 CAPLUS
DOCUMENT NUMBER: 58:15011
ORIGINAL REFERENCE NO.: 58:2477f-h,2478a
TITLE: Alkaloids of Cynoglossum latifolium. Latifoline and 7-angelylretronecine
AUTHOR(S): Crowley, H. C.; Culvenor, C. C. J.
CORPORATE SOURCE: Div. Organic Chem., C.S.I.R.O., Melbourne
SOURCE: Australian Journal of Chemistry (1962), 15, 139-44
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The alkaloid content of C. latifolium was low and variable in dried material (free base, 0.02-0.08; N-oxide, 0.00-0.13%) but higher in fresh (free-base, 0.12-0.15; N-oxide, 0.10-0.12%). Counter-current distribution between CHCl3 and 0.5N HCl of total base (35 g.), after zinc reduction of N-oxides, yielded 12.4 g. latifoline (I), C20H27O7N, m. 102-3°, [α]24D 57° (EtOH), RF 0.58 in upper phase from shaking BuOH with 5% AcOH, (picrate m. 173-4°), and 1.8 g. 7-angelylretronecine (II), m. 76-7°, [α]24D 49° (EtOH), RF 0.52 (picrate m. 179-80°). II gave retronecine (III) on hydrolysis, and 7-(2-methylbutyryl)-retronecanol (IV) on hydrogenolysis. Alkaline hydrolysis of I gave III, angelic acid, and a noncryst. mixture of acids. Over platinum oxide I absorbed 3 moles H, to give IV and latifolic acid (V), m. 165-6°, [α]D 94.0° (EtOH). Both I and V have infrared spectra typical of γ-lactones, and V is shown to be the γ-lactone of 3,4-dihydroxypentane-2,3-dicarboxylic acid by its nuclear magnetic resonance spectrum, which shows two methyl group doublets (corrected τ-values 8.72 and 8.50) and two methinyl quadruplets (6.69 and 5.32), indicating two MeCH groups with no H atom on the other atoms attached to the CH groups.
IT 50460-79-2 92350-64-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 50460-79-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-3-hydroxy-2,4-dimethyl-5-oxo-, [2S-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



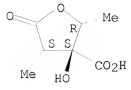
RN 92350-64-6 CAPLUS
CN Malic acid, 2-(1-hydroxyethyl)-3-methyl-, γ-lactone (7CI) (CA INDEX NAME)



IT 50460-94-1, Latifolic acid
(structure of)

RN 50460-94-1 CAPLUS
CN L-threo-Pentonic acid, 3-C-carboxy-2,5-dideoxy-2-C-methyl-, γ-lactone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 77 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:113136 CAPLUS
DOCUMENT NUMBER: 52:113136
ORIGINAL REFERENCE NO.: 52:19935g-i,19936a-i,19937a-h
TITLE: The synthesis of dl-protolichesterinic acid
AUTHOR(S): Van Tamelen, Eugene E.; Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of the American Chemical Society (1958), 80, 3079-86
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:113136

AB Me dl-dihydroprotolichesterinate (180 mg.), 0.024 g. Na, and 5.5 cc. MeOH refluxed 1 hr., poured into H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, the residue (0.129 g.) dissolved in 7 cc. MeOH, the solution treated with 1 cc. H2O containing 0.0304 g. NaOH, kept 5 days at room temperature, diluted with H2O, acidified with NaHSO4, and the precipitate recrystd. from glacial AcOH, washed with petr. ether, and recrystd. again from MeOH yielded 0.056 g. neodihydroprotolichesterinic acid (I), platelets, m. 97-8° (all m.ps. are corrected) I with CH2N2 gave the Me ester, m. 38-9° (uncor.). Me dl-isodihydroprotolichesterinate (0.31 g.) and 10.5 cc. absolute MeOH refluxed 5.5 hrs. with 0.00419 g. Na, treated with 1 cc. H2O, refluxed 6.5 hrs., cooled, diluted with H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, and the residue extracted with cold petr. ether left 0.070 g. I. C13H27COCH2CO2Me (II) (5 g.) and 2.9 g. powdered NaI added to 0.41 g. Na in 10 cc. absolute MeOH, the mixture treated with cooling during 10 min. with 3.0 g. BrCH2CO2Et, kept 2 days at room temperature, filtered, the residue washed with H2O, the filtrate poured into H2O, acidified and extracted with Et2O, and the extract worked up yielded 2.53 g. dialkylation product, C25H44O7, m. 42-3°. II (10 g.), 100 cc. dry C6H6, and 10 g. pyrrolidine, b. 86.5-87° refluxed 9 hrs. with the azeotropic removal of about 0.8 cc. H2O and evaporated gave 11.5 g. pyrrolidine enamine (III) of II, yellow liquid. III (11.5 g.), 100 cc. absolute MeOH, and 5.85 g. BrCH2CO2Et refluxed 29 hrs., and stirred overnight with 20 cc. H2O, the aqueous layer extracted with Et2O, and the combined organic layer and extract evaporated gave 10 g. brown oily C13H27COCH(CO2Me)CH2CO2Et (IV); a 10-g. portion in 50 cc. absolute MeOH treated with 8 cc. 1.0M NaBH4 in MeOH, allowed to stand 3 days, treated again with 11 cc. NaBH4 solution, allowed to stand 3 hrs., poured into H2O, acidified with NaHSO4, and extracted with Et2O, the extract washed, dried, and evaporated, the residual yellow oil dissolved with 7 g. KOH in 110 cc. 90% MeOH, allowed to stand 1 day at room temperature, cooled, filtered, the residue acidified with 5% HCl, digested 1 hr. at 70°, kept several hrs. at room temperature, filtered, dried (5.1 g.), and recrystd. from C6H6 yielded 4.8 g. 3-carboxy-4-oxoheptadecanoate (V), m. 80-3°. V (1 g.) treated with CH2N2 in Et2O and evaporated yielded 1.03 g. β-carbomethoxy-γ-tridecyl-γ-butyrolactone (VI), m. 68-70° (MeOH). (EtO)2CO (80 g.) and 8.6 g. butyrolactone refluxed at 125 mm., treated during 1 hr. with 2.39 g. Na in 56 cc. absolute EtOH while removing the EtOH simultaneously with the addition, the residual pale yellow, gelatinous mass poured into 60 cc. glacial AcOH and ice and extracted with 50 cc. Et2O, and the extract worked up yielded 4.1 g. α-carbethoxy-γ-butyrolactone(VII), b0.5, 106-9°. VII in EtOH treated with excess liquid NH3 gave HO(CH2)2CH(CONH2)2, m. 152.5-53° (EtOH). VI (3 g.) and 7.55 g. (EtO)2CO treated dropwise during 1 hr. with stirring under reflux at 125 mm. with 0.212 g. Na in 5.6 cc. absolute EtOH while removing the EtOH continuously, the resulting slush poured into 6 cc. glacial AcOH and ice and extracted with Et2O, and the extract worked up yielded 3.4 g. light red oil; a 0.79-g. portion chromatographed

on 12 g. silicic acid did not give the desired carbethoxylation product; a 2.37-g. portion in 20 cc. MeOH containing 1.27 g. KOH kept 5 days at room temperature, acidified with 5% HCl, filtered, and the residue washed with H2O, dried, and extracted with ligroine (b. 60-8°) left 1.4 g. material C18H32O4, m. 133-5°. C13H27CH:CHCO2H (VIII), m. 47-9° (aqueous EtOH), was prepared by the method of Myers (C.A. 46, 1438g) and separated in 45% yield from the by-product C14H29CH(OH)CO2H by extracting the crude mixture with petr. ether at room temperature, filtering, cooling to 0°, filtering again, evaporating, and recrystg. the residue from aqueous MeOH. VIII (5 g.) in 50 cc. Et2O treated with CH2N2 in Et2O until the yellow color persisted for 5 min. and evaporated on the steam bath gave 5.3 g. Me ester (IX) of VIII. trans-VIII (1.0 g.) in a few cc. CCl4 treated with about 8 cc. 5% CCl4-Br in small portions during 0.5 hr. and evaporated, the residual yellow oily paste dissolved in 10 cc. Ac2O, the solution treated with 0.5 g. powdered KOAc, refluxed 3 hrs., treated with iced H2O, and filtered, the residual creamy paste refluxed 0.5 hr. with 15 cc. 8% alc. KOH, the mixture cooled, poured onto 50 g. ice containing a slight excess of dilute H2SO4, and extracted with Et2O, the extract evaporated, and the residual pale yellow waxy solid triturated during several days at room temperature with a few cc. petr. ether gave 0.04 g. compound A, m. 88.5-9.5°; the filtrate from the isolation of compound A cooled in ice gave 0.30 g. impure compound B, m. 56-61.5°; the crude compound B treated with three 10-cc. portions ligroine at room temperature, the combined exts. concentrated to 10 cc., cooled to 15°, and centrifuged, and the precipitate washed with a little cold ligroine and recrystd. from ligroine at 10° yielded 10 mg. pure cis-2,3-epoxyhexadecanoic acid, flakes, m. 70.0-70.9°. (CF3CO)2O (21.2 cc.), 3.5 cc. 90% H2O2, and 25 cc. CH2Cl2 added with cooling dropwise during 40 min. to 10.6 g. IX, 56.5 g. Na2HPO4, and 70 cc. dry CH2Cl2, refluxed 0.5 hr., and stirred with 100 cc. H2O, the aqueous layer washed with 70 cc. CH2Cl2, and the combined organic layer and extract washed, dried, and worked up yielded Me tridecylglycidate (X) in 3 fractions: (1) b0.4 140-6°, 3.73g.; (2) b0.4 148-50°, 2.62 g.; (3) b0.4 150-2°, 3.73 g. X (0.2902 g.), 10 cc. dioxane, and 0.5 cc. 10% aqueous NaOH refluxed 1.5 hrs. under N, cooled, poured into iced H2O containing 5 cc. 5% HCl, and extracted with Et2O, the extract worked up, and the residual oil diluted with 8 cc. petr. ether, cooled, and filtered yielded 0.122 g. trans-tridecylglycidic acid, platelets, m. 86-7°. Na (0.485 g.) in 8 cc. absolute MeOH treated with 2.79 g. CH2(CO2Me)2, the mixture treated during 10 min. with stirring with 6.00 g. X in 10 cc. absolute MeOH, refluxed 4 hrs., cooled, poured into 150 cc. ice and H2O, acidified with 5% HCl, extracted with CHCl3, and the extract worked up gave 7.85 g. crude, pale yellow, oily product which chromatographed on silicic acid gave pure α,β- dicarbomethoxy-γ-tridecyl-γ-butyrolactone (XI), white wax. XI (2.1 g.) in 40 cc. MeOH treated with 5 cc. H2O containing 1.84 g. KOH, refluxed 3 hrs., kept overnight at room temperature, decanted, the oily residue dissolved in 50 cc. H2O, the solution acidified with 5% HCl to Congo red and filtered, and the residue dried (1.182 g.) and recrystd. from 20 cc. hot MeOH yielded 0.721 g. mono-K salt (XII) of α,β-dicarboxy-γ-tridecylbutyrolactone (XIII), powder, m. 124° (decomposition); the mother liquor poured into 100 cc. H2O, acidified with 5% HCl, extracted with Et2O, and the extract worked up gave 0.494 g. white material. XII (0.0394 g.) refluxed 0.5 hr. with 0.5 cc. 5% H2SO4, cooled, extracted with Et2O, and the extract worked up gave 0.0265 g. mixed diastereoisomers of V, m. 87.5-94.5°. XII (0.050 g.) in 5

cc. MeOH acidified with 5% HCl, diluted with H2O, extracted with Et2O, and the extract dried and evaporated under N at room temperature gave 0.036 g. XIII. XII

(0.372 g.) treated with 0.207 g. Et2NH and 0.126 g. 30% aqueous CH2O, diluted with 2 cc. MeOH, heated 1 min. on the steam bath, kept 1 day at room temperature, treated again with 0.126 g. 30% aqueous CH2O, allowed to stand 1 day,

diluted with a few cc. MeOH, evaporated, the residue evaporated twice with CHCl3,

the resulting solid kept overnight in 5 cc. CHCl3 and filtered, and the residue (0.114 g.) dissolved in glacial AcOH, treated with a few drops H2O, cooled to 15°, and filtered gave 0.061 g.

dl-protolichesterinic acid (XIV), m. 92.5-4.5° the filtrate from

the crude XIV K salt evaporated, the residual semisolid dissolved in 2 cc. dry C6H6, the solution kept 3 days at room temperature with 5 cc. MeI, filtered, evaporated

at about 40° under N, the residual crude oil (0.338 g.) dissolved

in 4 cc. MeOH, the solution treated with 5.5 cc. 5% aqueous NaHCO3, allowed to stand 3 days, diluted with H2O, extracted with Et2O, the aqueous solution acidified

with 5% HCl and extracted with Et2O, and the extract worked up yielded 0.0513 g.

(crude) XIV, m. 87.5-97.5°. Crude XIV (74 mg.) chromatographed on

5 g. silicic acid gave 29% purified dl-lichesterinic acid (XV), m. 114-15°, 42% XIV, m. 100.5-101.5°, and 11.8% less pure XIV, m. 98.5-100°. XIV (30 mg.) and 5 cc. Ac2O heated 1 hr. on the steam bath, cooled, diluted with H2O, and filtered yielded 21 mg. XV, m. 113-15° (AcOH). XIV (20 mg.) in 10 cc. glacial AcOH hydrogenated

over 50 mg. 10% Pd-C, filtered, diluted with H2O, the precipitate recrystd. from

AcOH, and the product extracted with boiling ligroine and recrystd. from AcOH yielded 9 mg. dihydro derivative of XV, m. 114-16°. XII (0.3835 g.), 3 cc. MeOH, 0.079 g. Me2NH.HCl, 0.0873 g. Me2NH, and 0.097 g. 30% aqueous CH2O kept 2 days at room temperature, filtered, treated with a few cc. MeOH, evaporated

in vacuo on the steam bath, this procedure repeated twice with the addition and removal of CHCl3, the residual waxy solid treated with 3 cc. dry C6H6 and 5 cc. MeI, the mixture kept 3 days at room temperature, filtered, and the residue (0.653 g.) recrystd. from glacial AcOH yielded 0.340 g. methiodide (XVI), platelets, m. 165° (decomposition); the filtrate evaporated under N, the residual yellow oil (0.126 g.) dissolved in 2 cc. MeOH, the solution treated 3 days at room temperature with 2.1 cc. 5% aqueous NaHCO3 and extracted with

Et2O, the aqueous phase acidified with 5% HCl and extracted with Et2O, the extract

dried and evaporated, and the residue (0.038 g.) extracted with ligroine and recrystd. from aqueous AcOH gave 0.010 g. V, m. 98-100°. MeOH (5 cc.) and 2.8 cc. 5% aqueous NaHCO3 added to 0.211 g. XVI, kept 3 days at room temperature, diluted with H2O, washed with CHCl3, acidified, extracted with CHCl3, and

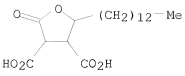
the extract worked up yielded 0.029 g. XIII, m. 92-5° (AcOH).

IT 51175-46-3 109815-40-9

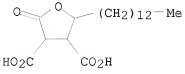
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 51175-46-3 CAPLUS

CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)

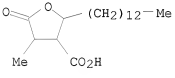


RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)

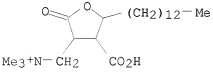


● K

IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
(isomers)
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



IT 118978-13-5P, Ammonium, (2,3-dicarboxy-4-hydroxyheptadecyl)trimethyl-, iodide, γ-lactone
RL: PREP (Preparation)
(preparation of)
RN 118978-13-5 CAPLUS
CN 3-Furanmethanaminium, 4-carboxytetrahydro-N,N,N-trimethyl-2-oxo-5-tridecyl-, iodide (1:1) (CA INDEX NAME)

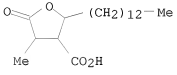


● I^-

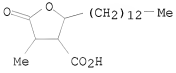
L14 ANSWER 78 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:51796 CAPLUS
DOCUMENT NUMBER: 51:51796
ORIGINAL REFERENCE NO.: 51:9566a-c
TITLE: Action of acetyl hydroperoxide on alkylfuryl alcohols
AUTHOR(S): Azanovskaya, M. M.; Pansevich-Kolyada, V. I.
SOURCE: Doklady Akademii Nauk SSSR (1956), 111, 1245-8
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Alkylfurylcarbinols were treated with 90-5% AcO2H in Et2O at 20-5° with 1:1 and 1:2 molar proportions of the reactants. With 1:1 mole ratio there were formed 2,3-epoxy-2-furylalkylcarbinols (alkyl group shown): Et, 48%, m. 69.5-71°; Pr, 62.7%, m. 57.5-9.5°; Bu, 72.6%, m. 82-3°; iso-Am, 30%, m. 60-1.5°. Treatment of the Bu compound with ZnCl2 or prolonged storage resulted in decomposition yielding BuCHO. When 2 moles of AcO2H is used for the oxidation only the Bu compound gave a trace of the above described monoepoxy compound The main bulk of the material from such reactions consisted of mixts. of aldehydes and acids. Thus the Bu compds. gave BuCHO, HCO2H, AcOH, and unidentified acids. The Et compound gave EtCHO, HCO2H, and AcOH, as well as unidentified acids. When the reaction was stopped before completion, appreciable amts. of monoepoxy compds. could be isolated.

IT 102180-12-1
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)

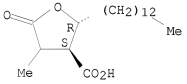


L14 ANSWER 79 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:51795 CAPLUS
DOCUMENT NUMBER: 51:51795
ORIGINAL REFERENCE NO.: 51:9565i,9566a
TITLE: Synthesis of protolichesterinic acid, dihydroprotolichesterinic acid, and lichesterinic acid methyl ester
AUTHOR(S): Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: (1957) 99 pp.;microfilm, $2.00; paper enlargement, $9.90 Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 20222
From: Dissertation Abstr. 17, 501
DOCUMENT TYPE: Dissertation
LANGUAGE: Unavailable
AB Unavailable
IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone 897946-24-6P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



RN 897946-24-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)- (CA INDEX NAME)

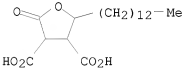
Absolute stereochemistry.



L14 ANSWER 80 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:34628 CAPLUS
DOCUMENT NUMBER: 51:34628
ORIGINAL REFERENCE NO.: 51:6517b-c
TITLE: Synthesis of (±)-protolichesterinic acid
AUTHOR(S): Van Tamelen, E. E.; Bach, S. R.
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Chemistry & Industry (London, United Kingdom) (1956) 1308
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

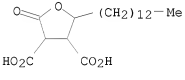
AB cf. C.A. 50, 6322a). A stereoselective synthesis of (±)-protolichesterinic acid (I) was carried out. Me 2-hexadecenoate with CF3CO3H yielded Me 2,3-epoxyhexadecanoate, b0.4 148-52°. Ring opening with di-Me malonate anion yielded, after spontaneous cyclization of the intermediate γ-hydroxy ester, α,β-dicarbomethoxy-γ-n-tridecyl-γ-butyrolactone. This on hydrolysis with hot MeOH-KOH was converted to the mono-K salt of the diacid, m. 124°, which with HCHO and Et2NH yielded I, m. 100.5-1.5°. Identification was confirmed by 3 separate tests.

IT 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)

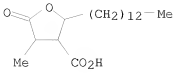


● K

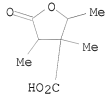
IT 51175-46-3, 1,1,2-Hexadecanetricarboxylic acid, 3-hydroxy-, γ-lactone
(and other derivs.)
RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



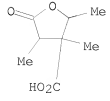
IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)


O
O
(CH2)12—Me
Me
CO2H

L14 ANSWER 81 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:9414 CAPLUS
DOCUMENT NUMBER: 51:9414
ORIGINAL REFERENCE NO.: 51:1996f-g
TITLE: The structure of sceleratine, an alkaloid from Senecio sceleratus
AUTHOR(S): de Waal, H. L.; Van Duuren, Benjamin L.
CORPORATE SOURCE: New York Univ., New York, NY
SOURCE: Journal of the American Chemical Society (1956), 78, 4464-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. preceding abstract Sceleranecic acid dilactone is shown on the basis of infrared data to be O.CO.CMe.CHMe.O.CO.C(CH2OH).CHMe. Sceleratinic dilactone is the corresponding CH2Cl analog.
IT 98558-94-2P, Succinic acid, 2-(1-hydroxyethyl)-2,3-dimethyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)
RN 98558-94-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2,3,4-trimethyl-5-oxo- (CA INDEX NAME)



L14 ANSWER 82 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:9413 CAPLUS
DOCUMENT NUMBER: 51:9413
ORIGINAL REFERENCE NO.: 51:1995i,1996a-f
TITLE: The structures of grantianine and sceleratine. A suggested biogenesis of the acids in the alkaloids from Senecio and Crotalaria species
AUTHOR(S): Adams, Roger; Gianturco, Maurizio
CORPORATE SOURCE: Univ. of Illinois, Urbana
SOURCE: Journal of the American Chemical Society (1956), 78, 4458-64
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Grantianine (I), the alkaloid from Crotalaria grantiana, has been reinvestigated. Grantianic acid, which is esterified with retronecine to form I, has been shown to be an oxidation product of trichodesmic acid. A reinterpretation of the results of de Waal, et al. (C.A. 48, 2702c), on sceleranecic acid dilactone has resulted in the postulation of the formula O.CO.CH.CHMe.C(CH2OH).CO.O.CMe2 for it, which conforms to those of the acid moieties of other Crotalaria alkaloids. Structure II is proposed for the alkaloid sceleratine. The possible existence of a common biogenetic pathway to the formation of the various acids, which when esterified with retronecine and related bases, provide the large class of pyrrolizidine alkaloids is discussed. I, m. 204-5°, [α]D30 50.6° (CHCl3), chromatographed with the upper layer of a mixture of equal vols. of BuOH and 5% AcOH on paper at 27 ± 1° gave the Rf value 0.45 (monocrotaline 0.40). I (0.050 g.) in 5 cc. 95% EtOH and 3 cc. glacial AcOH hydrogenated 7 min. under ambient conditions over 0.025 g. PtO2, the mixture filtered, the catalyst washed with EtOH containing 1% AcOH, and the combined solns. evaporated to dryness yielded 0.047 g. tetrahydro derivative (III) of I, white crystals, m. 242-2.5°, [α]D27 -56.8° (50% aqueous AcOH), Rf 0.29. The rotation solution (0.023 g. in 1.5 cc. solvent) acidified with 0.1 cc. concentrated HCl gave immediately the value [α]D27 -54.0° which did not change during 20 hrs. at room temperature; the Rf value remained 0.29 (only 1 spot). III treated with an equivalent amount picric acid in H2O gave the picrate, m. 195-6°. Whether an alkaloid reduction product is a salt where both ester linkages have been cleaved or where intramolecular salt formation with the cleavage of only 1 ester group had occurred can be determined in the following manner. A few mg. of the product is dissolved in 1-2 cc. H2O, the pH tested, and the solution treated with a few mg. Dowex 50 (H form): the 1st type of salt gives a pH change to more acidic values: no pH change is observed with the 2nd type.
IT 98558-94-2P, Succinic acid, 2-(1-hydroxyethyl)-2,3-dimethyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)
RN 98558-94-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-2,3,4-trimethyl-5-oxo- (CA INDEX NAME)



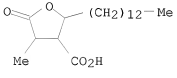
L14 ANSWER 83 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1956:31889 CAPLUS
DOCUMENT NUMBER: 50:31889
ORIGINAL REFERENCE NO.: 50:6322a-i
TITLE: Synthesis of dl-lichesterinic acid methyl ester
AUTHOR(S): Van Tameslen, Eugene E.; Osborne, Clyde E., Jr.; Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of the American Chemical Society (1955), 77, 4625-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The Me ester (I) of dl-lichesterinic acid O.CO.CMe:C(CO2H).CH(CH2)12Me (II) has been synthesized by the SO2Cl2 dehydrogenation of Me ester (III) of dl-dihydroprotolichesterinic acid (IV), which was prepared by the NaBH4 reduction of C13H27COCH(CO2Me)CHMeCO2Me (V). Various transformations encountered in the catalytic reduction of II and protolichesterinic acid (VI) are presented, and the possible biogenetic origins of these substances are discussed. C13H27COCH2CO2Me (VII), m. 38-9°, was prepared in 40% yield by the method of Stallberg-Stenhagen (C.A. 41, 4105d), filtering the crude product by suction with a rubber dam and recrystg. at 0° from petr. ether. VII (5.0 g.), 2.9 g. NaI, and 3.18 g. MeCHBrCO2Et added to 0.41 g. Na in 10 cc. absolute MeOH, the mixture heated a few min. on the steam bath, held 4-7 days at room temperature, poured into H2O, acidified with NaHSO4, and filtered, and the waxy filter residue recrystd. from 30 cc. ligroine (b. 60-8°) gave 4.35 g. C13H27 COCH(CO2Me)CHMeCO2Me (VIII), colorless prisms, m. 49-50°. VIII (5 g.) in 50 cc. absolute MeOH held 3 days at room temperature with 3.9 cc. 1.0M NaBH4 in MeOH, the mixture treated with an addnl. 5.5 cc. NaBH4 solution, allowed to stand 3 hrs., and poured into H2O, the mixture acidified with NaHSO4, the precipitated oil extracted into Et2O, the extract dried and evaporated, the oily residue refluxed 19 hrs. with 3.5 g. KOH in 55 cc. 90% MeOH, the precipitate filtered, dissolved in H2O, and acidified with 5% HCl, the crude precipitate extracted with petr. ether, and the insol. residue recrystd. from glacial AcOH yielded 1.70 g. IV, m. 114-15°; the filtrate of the hydrolysis mixture poured into a large excess H2O and acidified with NaHSO4, the crystalline precipitate dried and extracted with boiling ligroine (b. 60-8°) to remove some II, m. 84.5-5.0°, and the residue recrystd. from glacial AcOH yielded 9% dl-isodihydroprotolichesterinic acid (IX), m. 135-6°. IV treated with CH2N2 gave III, m. 62.0-2.5° (from MeOH). Similarly was prepared the Me ester of IX, m. 67.0-7.15°. d-VI hydrogenated in glacial AcOH at room temperature over 10% PdC, the mixture diluted with H2O, and the precipitate recrystd. from glacial AcOH yielded 60% d-IV, m. 103.5-4.5°; Me ester, m. 54.5-5.5°. VI (1.8 g.) hydrogenated in the same manner gave dl-IV, m. 109-16°. C13H27CH:CHCO2H (8.8 g.) in 500 cc. H2O containing 18.5 g. KOH cooled to 0° with stirring, the resulting suspension warmed to room temperature, treated with stirring during 4 hrs. with 2.50 g. Cl gas, and acidified with an equivalent amount H2SO4, the white solid precipitate dissolved in Et2O, the solution dried and concentrated, the residual pale yellow oil dissolved in 90 cc. ligroine, the solution cooled several days at 0-5°, and the crystalline deposit (2.3 g.) recrystd. from ligroine gave 1.7 g. chlorohydroxydecanoic acid, m. 75.7-6.2°; Et ester, m. 50.8-1.5°. III (200 mg.), 160 mg. SO2Cl2, and 10 mg. Bz2O2 in 0.5 cc. CCl4 refluxed 18 hrs., the solvent removed in vacuo, the residue

treated with H2O and 20 cc. Et2O, the Et2O layer dried and evaporated, the residue dissolved in 1 cc. EtOH, the solution filtered, and chilled, and the solid deposit dried and recrystd. from MeOH yielded 7-17% I, m. 49-50°. II (5 mg.) from equal parts of the optical antipodes treated with CH2N2 in Et2O yielded I, m. 51-2°. IV heated with Br in polyphosphoric acid at 120-40° and the resulting product treated with collidine gave an unseparable mixture of products. IV treated with N-bromosuccinimide and Bz2O2 gave crude material containing about 7% II. dl-I (9.6 mg.) in 2 cc. MeOH treated with 1 cc. 2.66 + 10-2M aqueous NaOH, the solution held 5 days at room temperature, acidified with NaHSO4, and filtered, the filter residue dissolved in ligroine, the solution filtered and evaporated, and the residue recrystd. gave dl-II, m. 83-4°. d-II (540 mg.) in 200 cc. glacial AcOH hydrogenated over 200 mg. PtO2, the mixture filtered, the filtrate diluted with H2O, and the precipitate extracted with boiling ligroine and recrystd. 3 times from glacial AcOH yielded 250 mg. C13H27CH(CO2H)CHMeCO2H (X), m. 135.5-6.5°. X (82 mg.) heated 1 hr. at 100° in a sealed tube with 0.4 cc. AcCl, the excess AcCl evaporated, and the residue recrystd. from ligroine, at -78° gave 57% anhydride of X, m. 34°.

IT 102180-12-1P, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

RN 102180-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



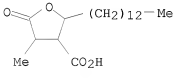
L14 ANSWER 84 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1951:39033 CAPLUS
DOCUMENT NUMBER: 45:39033
ORIGINAL REFERENCE NO.: 45:6691h-i,6692a-b
TITLE: Antibacterial effects of lichen substances. I. Comparative studies of antibacterial effects of various types of lichen substances
AUTHOR(S): Shibata, Shoji; Miura, Yoshiaki; Sugimura, Hisako; Toyoizumi, Yuri
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Yakugaku Zasshi (1948), 68, 300-3
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. preceding abstract The relation between the chemical structure of usnic acid and its antibacterial effects described in previous papers was discussed. Comparatively powerful antibacterial activities against gram-pos. bacteria were found in lichesterinic acid and its derivs. and in depsides from orcinols having large alkyl radicals. No antibacterial activities were found in fatty acids of the caperatic acid type, depsides of the β-orcinol series, depsidones, and endocrocin related to anthraquinone. None showed any activity against gram-neg. bacteria. The highest dilns. inhibiting growth of M. tuberculosis (avian type) and Staph. aureus, resp., were: protolichesterinic acid −, 1:80,000; l-lichesterinic acid 1:40,000, 1:160,000; l-dihydroprotolichesterinic acid 1:80,000, 1:80,000; caperatic acid −, 1:5,000; rangiformic acid −, < 1:5,000; zeorin −, < 1:5,000; lecanoric acid −, < 1:5,000; divaricatic acid 1:10,000, 1:80,000; sphaerophorin −, 1:80,000; anziaic acid −, 1:80,000; perlatolinic acid 1:40,000, 1:80,000; olivetoric acid 1:10,000, 1:20,000; sekikaic acid 1:10,000, 1:80,000; ramalinolic acid −, 1:20,000; boninic acid −, 1:10,000; atranorin −, < 1:5,000; thamnolic acid −, < 1:5,000; lobaric acid −, 1:20,000; salazinic acid −, 1:5,000; psoromic acid −, 1:5,000; fumarprotocetraric acid −, < 1:5,000; pannarin −, < 1:5,000; endocrocin −, <1:5,000.

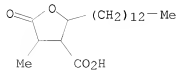
IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone
(antibacterial effects of)

RN 102180-12-1 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



L14 ANSWER 85 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1949:6300 CAPLUS
DOCUMENT NUMBER: 43:6300
ORIGINAL REFERENCE NO.: 43:1322b-f
TITLE: Lactone aliphatic acids as antibacterial agents
AUTHOR(S): Cavallito, Chester J.; Fruehauf, Dorothy M.; Bailey, John H.
SOURCE: Journal of the American Chemical Society (1948), 70, 3724-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB A study has been made of the relationship between lactone structure and antibiotic activity. The Na salt of α-carbethoxybutyrolactone (18 g.) in 250 cc. absolute EtOH and 0.1 mol. of the alkyl bromide were refluxed 4 hrs., the reaction mixture poured into 500 cc. H2O, extracted with three 150-cc. portions of CHCl3, and the residue saponified with 8.4 g. KOH in 150 cc. EtOH; the yields of the substituted α-carboxybutyrolactones, H2C.CH2.CR(CO2H).CO.O, were from 20 to 45% (R is given): C10H21 m. 75-7° (m.ps. corrected), η (in 0.1 M K phosphate buffer at pH 7; acid concentration 3 + 10-5 millimol./cc.) 70.3; C12H25 m. 78-9°, ε 68.1; C13H27 m. 69-70°, η 43.3; C14H29 m. 82-3°, η 35.0 (γ-Me derivative m. 64-7°, η 33.2); C16H33 m. 80-2°, η 41.4 (γ-Me derivative m. 60-3°, η 37.6). l-Protolichesterinic acid (I) (1.5 g.) and 1.5 g. l-cysteine-HCl in dilute NaHCO3 (pH 7), kept 20 hrs. at 25° and the solution strongly acidified with HCl, give 1 g. of the l-cysteine derivative (II) of I, m. 185-8° (decomposition); the addition appears to be through the SH group. Data are given for the min. bacteriostatic concentration for Streptococcus hemolyticus C203, Staphylococcus aureus 209, Clostridium welchii, Bacillus typhi, and B. tuberculosis ranae and H37Rv for the above lactones, I, II, l-lichesterinic acid, l-dihydroprotolichesterinic acid, and chaulmoogric acid. The antibacterial activity of I is related to its effect on η and not to any significant extent on the unsatd. system. II is much less inhibitory to bacteria than is I. Of the lactones, the C14 chain was optimum in contributing to the antibacterial activity and the γ-Me derivative has about the same activity. The lactone aliphatic acids are more compatible with complex media than are the aliphatic monocarboxylic and malonic acids and are more soluble at neutrality.
IT 102180-12-1, Succinic acid, 2-(1-hydroxytetradecyl)-3-methyl-, γ-lactone of l-
(bacteriostatic action of)
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



L14 ANSWER 86 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1939:59734 CAPLUS
DOCUMENT NUMBER: 33:59734
ORIGINAL REFERENCE NO.: 33:8593d-f
TITLE: Constituents of Nephromopsis stracheyi f. ectocarpisma Hue. II. Constitution of nephromopsinic acid
AUTHOR(S): Asano, Mituzo; Yasusumi, T.
SOURCE: Yakugaku Zasshi (1939), 59, 377-83
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

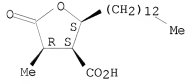
AB cf. C. A. 29, 5072.6. Nephromopsinic acid (I) (2.5 g.) when boiled for 1.5 hrs. with 40 cc. 5% alc. KOH, treated with 6.9 g. AgNO3 in alc. and heated for 2 hrs. at 50° with 15 g. MeI gave nephromopsinic methyl ester (II), m. 59-60°. Hydrolysis of II gave dihydro-l-protolichesterinic acid, C19H34O4, m. 103-5°. Et pelargonoylacetate (6 g.), NaOEt and 5 g. MeCHBrCO2Et when heated in the sealed tube at 120° for 5 hrs. gave Et α-methyl-α'-pelargonoylsuccinate (III), b3 158-62°. Reduction of 20 g. III with Na-Hg gave 1 g. α-methyl-γ-octylpelargonic acid, C14H24O4, m. 112-14°; hydrolysis of the Et ester gave α-methyl-α'-nonylidenesuccinic acid, C14H24O4, m. 132-4°. Et myristinoylacetate (7 g.), NaOEt and 4.3 g. MeCHBrCO2Et when heated in the sealed tube at 120-30° for 4 hrs. gave Et methylmyristionylsuccinate (IV). Reduction of 34 g. IV with Na-Hg gave a small amount of α-methyl-γ-tridecylpelargonic acid, C19H34O4, m. 134-6°.

IT 493-45-8, Nephromopsinic acid (and derivs.)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.

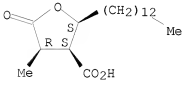


L14 ANSWER 87 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1939:59733 CAPLUS
DOCUMENT NUMBER: 33:59733
ORIGINAL REFERENCE NO.: 33:8593b-d
TITLE: Preparation of acetyl-5-fluorosalicylic acid
AUTHOR(S): Suter, C. M.; Weston, Arthur W.
SOURCE: Journal of the American Chemical Society (1939), 61, 2317-18
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 33:59733

AB Carbonation of the Mg derivative of 2-bromo-4-fluorophenetole gives 64.5% of 2-ethoxy-5-fluorobenzoic acid, m. 65.5-6.5°; refluxing with HI (d. 1.7) for 10 hrs. gives 87% of 5-fluorosalicylic acid (I), m. 178.5-9.5°; FeCl3 gives a purple-violet color; the Me ester has the "oil of wintergreen" odor; Ac derivative (II), m. 130-1°, 56% yield. I is approx. twice as toxic as the F-free acid and II is about 50% more toxic than aspirin. 5-Chlorosalicylic acid has the same germicidal action as the parent acid.

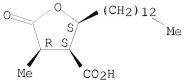
IT 493-45-8, Nephromopsinic acid
(and derivs.)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)-
(CA INDEX NAME)

Absolute stereochemistry.

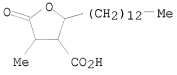


L14 ANSWER 88 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1939:14245 CAPLUS
DOCUMENT NUMBER: 33:14245
ORIGINAL REFERENCE NO.: 33:2125a-f
TITLE: Constitution of nephromopsinic acid. II
AUTHOR(S): Asano, Mitizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1939), 72B, 35-9
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 29, 5072.6. When nephromopsinic acid, C19H34O4 (I), which is probably a diastereomer of dihydroprotolichesterinic acid, RC4H.C3H(CO2H).C2HMe.ClO.O (II, R = C13H27), is heated with 2 equivs. of alc. KOH so that the lactone ring is opened and is then treated with AgNO3 it gives a gray-black Ag salt which with MeI yields the Me ester, m. 59-60°, of I, identical with that obtained with CH2N2. On the other hand, saponification of this ester with alc. KOH does not regenerate the original I but I-II, m. 103-5°. As II is formed by hydrogenation of protolichesterinic acid, it must be assumed that the 2-C atom of II is racemized. It follows that alkaline saponification of I opens the lactone ring, to be sure, but does not racemize the 2-C atom; when, however, its ester is saponified, the 2-C atom is first enolized and on acidification II is formed. α-Methyl-γ-alkylparaconic acids (II) were synthesized according to the scheme RCOCH2CO2Et + MeCHBrCO2Et (III) → RCOCH(CO2Et)CHMeCO2Et (+ Na-Hg) → II. From 6 g. Et pelargonoylacetate (IV), b16 149-51°, b2 115°, with III and Na in alc. at 120° was obtained 8 g. di-Et α-methyl-α'-pelargonoylsuccinate (V), b3 158-62°, which gives a faint brown color with alc. FeCl3. The residue from the distillation of IV solidified on long standing and yielded from AcOH tablets of 6-octyl-3-pelargonoylpyronone, m. 70-1°, insol. in alkali and giving no color with FeCl3. V (20 g.) in alc. and water treated in the course of 3 days with Na-Hg with occasional addns. of AcOH to tone down the alkalinity gave about 8 g. acid products which on esterification yielded 1 g. α-methyl-γ-octylparaconic acid (VI), m. 112-14°, and a mixture of esters separated into 4 g. b2 130-60° (VII) and 2 g. b2 164-70° (VIII). Saponification of VII yielded α-methyl-γ-ketolauric acid, m. 62-3° (semicarbazone, m. 125-6.5°), and VIII gave VI. Heated with Na in alc. at 90-100° and then saponified with 5% KOH VIII yielded α-methyl-α'-nonylidenesuccinic acid, m. 132-4°, which immediately decolorized KMnO4. Et myristoylacetate (IX), b3 165-70°; in its distillation there remained a considerable residue of 6-tridecyl-3-myristoylpyronone, m. 85.5-7°, which with HI (d. 1.7) at 160-70° yielded ditridecylpyronone, m. 65-6°. α'-Myristoyl homolog of V (34 g. from 28 g. IX), brownish oil, gave with Na-Hg lichesterylic acid, m. 80-3°, and a little (0.1 g.) of the γ-tridecyl homolog of VI, m. 143-6°.
IT 493-45-8, Nephromopsinic acid
(and derivs.)
RN 493-45-8 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

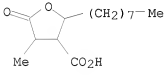
Absolute stereochemistry.



IT 102180-12-1P, Succinic acid,
α-(1-hydroxytetradecyl)-β-methyl-, γ-lactone
854909-07-2P, Succinic acid,
α-(1-hydroxynonyl)-β-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)
RN 102180-12-1 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl- (CA INDEX NAME)



RN 854909-07-2 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-2-octyl-5-oxo- (CA INDEX NAME)



L14 ANSWER 89 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1937:21713 CAPLUS
DOCUMENT NUMBER: 31:21713
ORIGINAL REFERENCE NO.: 31:3028h-i,3029a-i
TITLE: Lichen substances. LXXVII. The lichen aliphatic acids from Nephromopsis endocrocea
AUTHOR(S): Asahina, Yasuhiko; Yanagita, Masaiti; Sakurai, Y.
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1937), 70B, 227-35
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB It had been shown (C. A. 29, 7308.5) that Nephromopsis endocrocea Y. Asahina yields, in addition to the yellow pigment endocrocin, a colorless aliphatic acid (I) and a neutral substance (II). I, which was apparently a homogeneous lactonic acid, m. 93-5°, [α]D20 25.46°, proved to be really a mix. of 2 acids, for with KMnO4 it gave lauric acid and a saturated monobasic lactonic acid C17H30O4, designated nephrosteranic acid (III), and on ozonolysis yielded a considerable amount of HCHO, indicating the presence of a vinyl group (Clemo and MacDonald, C. A. 29, 7939.2). If I is heated with Ac2O, it gives an acid (IV), m. 112°, [α]D24 33.75° (CHCl3), stable toward cold KMnO4 but partly oxidized to lauric acid when heated, leaving III. With boiling alkali IV partially changes into a ketonic acid, nephrosterylic acid, C16H30O3 (V), whose oily oxime gives on Beckmann rearrangement an amide which can be cleaved to undecylamine, m. 20° (Bz derivative, m. 57°), and pyrotartaric acid, m. 112°. On dry distillation IV gives, along with III, an unsatd. lactone, C16H28O2 (VI), which is hydrolyzed by alkali to V; it must therefore be the enol lactone of V and is called nephrosterylolactone. These facts show that III is an original component of I which remains unchanged in all the above reactions. The other (unsatd.) component, which is designated nephrosterinic acid (VII), is reminiscent of protolichesterinic acid (C. A. 26, 5067). To sep. III and VII, I was treated with semicarbazide, which gave, together with III, a semicarbazino compound, C18H33O5N3 (VIII); the free VII could not be regenerated from VIII, but on the assumption that the semicarbazide adds at the vinyl double bond, VII would have the composition C17H28O4. VII was also obtained as a Hg(OH) Cl compound (IX) by treating I with Hg(OAc)2 and then with NaCl; demercurization of IX yielded no well defined product, however. A sharp separation of III and VII was effected by chromatography on Al3O3, the unsatd. VII being retained in the upper part of the Al2O3 while III accumulated in the lower part. On catalytic hydrogenation, the mixture I was completely converted into III; III is therefore a dihydro derivative of VII. VII is accordingly assigned the structure shown in the accompanying formula. By rearrangement it changes into isonephrosterinic acid (X) which on distillation loses CO2 and gives VI. On saponification with alkali, both X and VI yield V, C11H23COCH2CHMeCO2H, whose structure was established by synthesis as well as by the Hofmann rearrangement of its oxime (see above). II is very similar to, perhaps identical with caperin (J. prakt. Chemical 58, 409(1898)); it gives sterol-like color reactions, a property which has not been reported for caperin. III (0.3 g. from 1 g. I in 10% KOH treated with saturated KMnO4 to a permanent violet color), m. 95°, is recovered unchanged when boiled 3 hrs. in 10% KOH and acidified. V, m. 74°, soluble without color in Na2CO3; semicarbazone, m. 117°. VI (2.5 g. from 5 g. IV heated at 200-10° under 15 mm. until the evolution of CO2 ceases and then distilled at 210-30°), b3 185-9°, decolorizes KMnO4. VIII (0.4 g. from 1 g. I), sinters around 150°, decomposes 183-4°, is quite stable to KMnO4 in acetone. IX, m. 95°, very stable to HCl, gives in alc. AcOH HgS with H2S but the filtrate yields only amorphous products. VII, m.

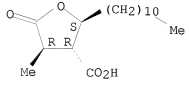
96°, [α]D10 10.81° (CHCl3), instantly decolorizes KMnO4 in acetone. X (0.05 g. from 0.12 g. VII heated 1 hr. in Ac2O at 105°), m. 113°, [α]D11 32.98° (CHCl3), stable to KMnO4 in acetone. Et laurinoylacetate (XI), from Et laurinoylacetoacetate and NH4OH, b10 173-5° gives with PhNHNH2 phenylundecylpyrazolone, sandy powder becoming discolored at 205° and carbonizing around 240°. Heated 4 hrs. in alc. at 120° with Na and MeCHBrCO2Me, XI yields a light yellow oil, b4 180-90°, consisting chiefly of Me Et methyllaurinoylsuccinate, which, heated 8 hrs. with HI (d. 1.7) on the water bath, gives α-methyl-β-laurinoylpropionic acid (= V). II, (C12H2O3)n, m. 248°, [α]D18.5 -100.2° (CHCl3), insol. in KOH, gives no color in alc. with either FeCl3 or bleaching powder, dissolves in hot concentrated H2SO4 with red-brown color changing to dirty green; the CHCl3 solution with a few drops Ac2O and 1 drop concentrated H2SO4 becomes blue-violet, then green.

IT 480-71-7P, Nephrosteranic acid
RL: PREP (Preparation)
(preparation of)

RN 480-71-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-undecyl-, (2S,3R,4R)-(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 90 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1936:22403 CAPLUS
DOCUMENT NUMBER: 30:22403
ORIGINAL REFERENCE NO.: 30:2945i,2946a-g
TITLE: Lichen substances. LXII. Constituents of Cetraria islandica Ach.
AUTHOR(S): Asahina, Yasuhiko; Yanagita, Masaiti
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1936), 69B, 120-5
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

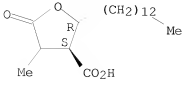
AB cf. C. A. 30, 1041.1. Asano (C. A. 26, 5067) established the structures of protolichesterinic (I) and lichesterinic acid (II), but as he worked not with Cetraria islandica Ach. (III) but with a lichen now considered to be an independent species, C. tenuifolia (Retz.) Howe (IV), the authors undertook a study of the true III, gathered on Mt. Asibetu and morphologically identical in all respects with the European lichen. It contained about 4% of a fatty acid mixture, m. around 90°, [α]D20 -45.62° (CHCl3), from which d-I was readily isolated. The mother liquor then yielded a strongly l-rotatory isomer, l-alloprotolichesterinic acid (V), which gave l-II with hot Ac2O and a pyrazoline derivative with CH2N2, and hence must be structurally identical with I. Heating the fatty acid mixture with Ac2O gave, as expected, dl-II. IV yielded l-I. The fumaroprotocetraric acid, however, which is always found in the European III and in IV, could not be detected in the Japanese III. Theoretically, I has 4 possible different configurations (2 pairs of optical antipodes). There is no reason for assuming a change in the configuration at C atom 4 when I changes into II; l-I would then differ from l-V only in the configuration at C atom 3. Hydrogenation of the I gives, theoretically, 2 dihydro derivs. each, the 8 isomers forming 4 pairs of optical antipodes. Whether the dihydro derivs. obtained from l-I, d-I and l-V are homogeneous or mixts. of 2 diastereomers has not yet been established. d-I, m. 106°, [α]D20 12.07° (CHCl3). V, m. 88°, [α]D23 -56.34° (absolute alc.), [α]D20 -49.53° (CHCl3), instantly decolorizes KMnO4 in acetone. Compound, C21H36O4N2, from V and CH2N2, m. 68-9°, [α]D18 -73.69°, stable toward KMnO4 in acetone. l-II, m. 123°, [α]D20 -25.06° (CHCl3). Dihydro derivative of l-V, m. 92-3°, stable toward KMnO4, [α]D20 -7.41° (CHCl3). l-I, m. 106°, [α]D18 -12.12° (CHCl3); dihydro derivative, m. 106°, [α]D18 -30.96° (CHCl3); pyrazoline derivative, m. 54-5°, [α]D18 -183.1° (CHCl3). Dihydro derivative of d-I, m. 106°, [α]D15 34.60° (CHCl3); pyrazoline derivative, m. 54-5°, [α]D18 190.60°.

IT 249647-94-7P, Protolichesterinic acid, dihydro-
897946-24-6P, Alloprotolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)

RN 249647-94-7 CAPLUS

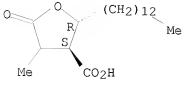
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 897946-24-6 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-
(CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 91 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1935:39202 CAPLUS
DOCUMENT NUMBER: 29:39202
ORIGINAL REFERENCE NO.: 29:5072f-i
TITLE: Constituents of Nephromopsis stracheyi f. ectocarpisma Hue. I
AUTHOR(S): Asano, Michizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1935), 68B, 995-7
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

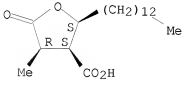
AB Extraction of the lichen with ether yields, with 0.03% usninic acid, 1% l-lichesterinic acid and some caperatic acid, 2 new acids, 0.2% of nephromopsinic acid (I), C19H34O4, m. 137°, and an acid C19H30O4 or C19H32O4 (II), m. 106-7°. I is the lactone of a saturated dibasic HO acid (Me ester, m. 60-1°), which with KMnO4 gives a little of a higher fatty acid, and with HI and red P in sealed tubes yields α-methyl-α-tetradecylsuccinanil, m. 63.5-4.5°. I might therefore be α-methyl-λ-tridecylparaconic acid (dihydroprotolichesterinic acid) (III) or tetradecylparaconic acid. Since, however, α-methyl-α'-tetradecylsuccinic acid has been prepared from III (see preceding abstract), I is probably a stereoisomer or diastereomer of III. II immediately decolorizes KMnO4 in AcOH. Its properties agree quite well with those of protolichesterinic acid (IV), but it depresses the m. p. of both d- and l-IV, and with CH2N2 it forms only the Me ester, m. 38-40°, no N-Me derivative

IT 493-45-8P, Nephromopsinic acid
RL: PREP (Preparation)
(preparation of)

RN 493-45-8 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2S,3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 92 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1935:39201 CAPLUS
DOCUMENT NUMBER: 29:39201
ORIGINAL REFERENCE NO.: 29:5072d-f
TITLE: Constituents of Iceland moss. V. Reduction of di-hydroprotolichesterinic acid and lichesterinic acid
AUTHOR(S): Asano, Michizo; Azumi, Tiaki
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1935), 68B, 991-4
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

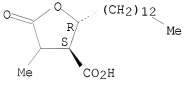
AB Cf. C. A. 26, 5067. λ-Isostearic acid (I), from lichesterinic acid with HI and red P (Boehm, Arch. Pharm. 241, 1 (1903)), m. 48-9°; amide, m. 104-4.5°; anilide, m. 86-6.5°; p-toluide, m. 82-3°. Lichesterylic acid with $N_2H_4.H_2O$ gives 4-methyl-6-tridecylpyridazinone, m. 66°, which with NaOEt at 170-80° smoothly yields I. I was also synthesized by condensing $MeCH(CO_2Et)_2$ with NaOEt and pentadecyl iodide to di-Et methylpentadecylmalonate, yellowish oil, b2 197-207°, saponifying the ester to the free acid, m. 95.5-6.5°, decomposing about 175°, and decarboxylating the latter at 170-80°. There can be no doubt, therefore, that I is α-methylheptadecanoic acid. Dihydro-d-protolichesterinic acid, m. 104-6° (Me ester, m. 51.5-2.5°), heated with HI and red P in a sealed tube and then reduced with Zn and AcOH, gives α-methyl-α'-tetradecylsuccinic acid, m. 133-5°.

IT 249647-94-7P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)

RN 249647-94-7 CAPLUS

CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.



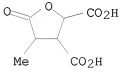
L14 ANSWER 93 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1931:16514 CAPLUS
DOCUMENT NUMBER: 25:16514
ORIGINAL REFERENCE NO.: 25:1832f-i,1833a-i
TITLE: Syntheses in the field of the santonin derivatives
AUTHOR(S): Chichibabin, A. E.; Shchukina, M. N.
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1930), 63B, 2793-806
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB This paper is published because of the appearance of the communications of Clemo, Haworth and Walton (C. A. 24, 4046) and of Berg (C. A. 24, 4300). The method chosen for the synthesis of santonin and related substances is closely analogous to that used for the synthesis of pilopic acid (C. A. 24, 3015). Succinic esters and their homologs are condensed with oxalic esters to oxalosuccinic esters, R'O2CCHRCH(CO2R')COCO2R', which are reduced to the HO esters, R'O2CCHRCH(CO2R')CH(OH)CO2R', and these on heating yield the lactonic acid esters, O.CO.CHR.CH(CO2R').CHCO2R' which contain 3 asym. C atoms and may therefore exist in 4 optically inactive stereoisomeric forms. By condensation of the anhydrides or chloroanhydrides of these lactonic acids with aromatic compds. (especially p-xylene and 2,5-Me2C6H3OMe) it was planned to prepare the products of incomplete condensation, 2,5-Me2C6H3COR'' (I) and 2,5,4-Me2(MeO)C6H2COR'' (II) (R'' = -CH.O.CO.CHR.CHCO2H), and those of complete condensation (III and IV) (IV = III with Me2(MeO)C6H instead of Me2C6H2). I and II on reduction should yield the dibasic acids Me2C6H3CH2CH2CH(CO2H)CHRCO2H (V) and Me2(MeO)C6H2CH2CH2CH(CO2H)CHRCO2H (VI) which by ring closure should give the tetrahydronaphthalene derivs. VII and VIII. Reduction of the ketone C:O group in VII and VIII and subsequent lactone formation should give compds. with structures (IX and X) which, when R = Me, have been shown by the work of C., H. and W. to be the structures of hyposantonin and desmotroposantonin Me ether. IX and X are also obtained by the method successfully used by C., H. and W., viz., ring closure of VII and VIII to the unsatd. lactones, XI and XII, and reduction. Reduction of the two ketone C:O groups in III and IV should give compds. (XIII and XIV) having the structures which recently have usually been assigned to hyposantonin and desmotroposantonin Me ether. Saponification of the MeO group in X and XIV would give the compds. (XV and XVI) having the 2 structures which have been given to desmotroposantonin. XIII and XIV can also be obtained in a more round-about way: reduction of I and II to Me2C6H3CH2R'' (XVII) and Me2(MeO)C6H2CH2R'' (XVIII) (R in R'' (see above) = Me), ring closure to the tetrahydronaphthalene derivs. (XIX and XX) and the reduction of the C:O groups to CH2. All these syntheses might be rendered difficult by the presence of the 3 asym. C atoms but it was hoped that the intermediate products corresponding to the stable hyposantonin and desmotroposantonin might also be stable and therefore the most easily formed modifications. The work has not yet been completed and the results so far obtained are published now to reserve the right of further investigation along this new broad road to the synthesis of santonin-like lactones. From EtO2CCHMeCH2CO2Et, (CO2Et)2 and NaOEt was obtained 80-90% EtO2CCHMeCH(CO2Et)COCO2Et (probably a mixture of stereoisomers), converted by reduction with amalgamated Al in moist Et2O into 85% of a mixture of esters of 3 stereoisomeric HO acids. On distillation in vacuo elimination of EtOH and lactone formation occurred and 200 g. of the reduction product after 15 fractionations yielded 88 g. liquid ester b13 182-3°, d20 1.1717, nD1.4498, 18 g. b13 186-7°, d20 1.1747, nD20 1.4507 and 13 g. solid ester, b13 200-4°, m. 70°. Of these di-Et 3-methylbutanolide-1,2-dicarboxylates, the first yielded with boiling HCl a free acid m. 179-82°, which with AcCl gave, along with dimethylmaleic anhydride, the anhydride, m. 162°; anilide, from the

anhydride and boiling PhNH2, m. 212-4°. The ester b13 186-7° gave an acid m. 186°, which strongly depressed the m. p. of the preceding acid and was for the most part unchanged by boiling AcCl, the small quantity which did react giving the above anhydride. The 2 acids are apparently cis-trans isomers. The solid ester gave an acid m. 185°, forming with AcCl an anhydride m. 201° which partly isomerizes into the 162° anhydride on distillation in vacuo and yields the same anilide with PhNH2. The 162° anhydride with p-xylene and AlCl3 gave the acid I, m. 171-3°, converted by heating 5 min. in concentrated H2SO4 on the H2O bath into an isomer m. 150°, which is obtained directly from the chloroanhydride of the 181-2° acid with p-xylene and AlCl3. I and its isomer with amalgamated Zn and concentrated HCl gave the compound V, m. 161-3°, but with amalgamated Zn and AcOH they yielded a compound 2,5-Me2C6H3COCH2CH(CO2H)CHMeCO2H, m. 169-72°, which is reduced to V by the Clemmensen method. The chloroanhydride, m. 182° (decomposition), of I, heated at 160-85°, yields the diketone III, light yellow, m. 137-9°, reacts neutral to litmus, soluble in boiling 10% but only difficultly in 0.1 N NaOH. The 162° anhydride with 2,5-Me2C6H3OMe gives the ketolactonic acid II, m. 207-8° (together with a small quantity of a substance m. 156°), which is reduced by the Clemmensen method to the compound VI, m. 131°, converted by demethylation with HI into the crystalline product from which was obtained, by the method of C., H. and W., their unsatd. lactone m. 250-2°.

IT 859081-04-2, 1,2,3-Butanetricarboxylic acid, 1-hydroxy-, γ-lactone
(isomers and derivs.)

RN 859081-04-2 CAPLUS

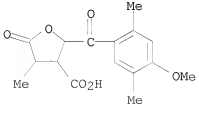
CN INDEX NAME NOT YET ASSIGNED



IT 856164-44-8P, Succinic acid, α-(α-hydroxy-4-methoxy-2,5-dimethylphenacyl)-β-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

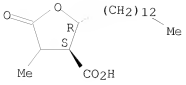
RN 856164-44-8 CAPLUS

CN Succinic acid, α-(α-hydroxy-4-methoxy-2,5-dimethylphenacyl)-β-methyl-, γ-lactone (3CI) (CA INDEX NAME)



L14 ANSWER 94 OF 94 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1928:37595 CAPLUS
DOCUMENT NUMBER: 22:37595
ORIGINAL REFERENCE NO.: 22:4470g-i,4471a-c
TITLE: Constitution of protolichestearic acid. I
AUTHOR(S): Asahina, Y.; Asano, M.
CORPORATE SOURCE: Tokyo Imp. Univ.
SOURCE: Yakugaku Zasshi (1927), No. 539, 1-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB By Et2O extraction of Cetraria islandica Ach. f. anguslifolia, Kraplh., a subalpine moss in Japan, l-protolichestearic acid (I), C19H32O4, m. 105°, [α]D27 -12.7l°, was isolated in 1.3% yield. It is the optical antipode of the d-acid found in European lichens. I, H2 and Pt black gave dihydroprotolicheslearic acid, C19H34O4, m. 101°. I and H2NCONHNH2 gave the semicarbazone, m. about 140°. These reactions indicate the presence of a double bond in α,β-position to the CO group. Oxidation of I with KMnO4 gave myristic acid, while the oxidation with O3 and subsequent decomposition with H2O gave besides HCO2H and (CO2H)2, α-hydroxypentadecylic acid, C14H28(OH)CO2H. Heating of I with Ac2O resulted in an isometic change and gave l-lichestearic acid (II), C19H32O4, m. 124°, [α]D25 -32.66°. Heating of II with 10% KOH gave with CO2 evolution, lichesteryl acid (III), C18H34O3, m. 83-4°. III has previously been prepared by Sinnhold (Ann. 55, 144), but the nature of the third O atom remained unexplained. Heating of the oxime of III with H2SO4 resulted in Beckmann rearrangement and gave an acid amide (IV) C18H35(NO3), m. 102°. IV and concentrated HBr in a closed tube gave tridecylamine and methylsuccinic acid. The above reactions show that III has 2 possible structures RCOCH2CHMeCO2H or RCOCHMeCH2CO2H (R = Me(CH2)12-). Heating of II in a vacuum at 20 mm. and 210° gave lichesteryl lactone (V), b. 207°, which on saponification with KOH gave III. V, H2 and Pd-BaSO4 gave the dihydro derivative of V, m. 37-8°, while V, O3 and H2O gave AcOH as a decomposition product. Contrary to the view of Boehm (Arch. Pharm. 241, 1) V is therefore unsatd. The above reactions show that the relation of III to V is like that of levulinic acid to angelic lactone. Hence V has one of the following 4 possible structures: (a) R-CH.CH:CMe.CO.O, (b) R-C:CH.CHMe.CO.O, (c) RCH.CMe:CH.CO.O, (d) RC:C.Me.CH2.CO.O. But the fact that the ozonide of V gave AcOH instead of (CO2H)2 favors the structure (a) for V, while III should have the structure, RCOCH2CH(Me)CO2H. I, therefore, has one of the 2 possible structures, RCH.CH(CO2H).C(:CH2)CO.O or RCH.C(CO2H):CMe.CO.O. Since the ozonide of I gave HCO2H and (CO2H)2 instead of AcOH, the former structure is preferred. From the fact that I did not give III, but II gave III by saponification with an alkali, the following structure is assigned for III.
IT 249647-94-7P, Protolichesterinic acid, dihydro-
RL: PREP (Preparation)
(preparation of)
RN 249647-94-7 CAPLUS
CN 3-Furancarboxylic acid, tetrahydro-4-methyl-5-oxo-2-tridecyl-, (2R,3S)-rel- (CA INDEX NAME)

Relative stereochemistry.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O
R
S
(CH2)12
Me
Me
CO2H

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     FILE 'CAPLUS' ENTERED AT 18:49:11 ON 20 JUL 2009
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L7             STRUCTURE UPLOADED
L8          100 S L7 FULL

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L10          45 S L6 NOT L9

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L12         150 S L11 FULL

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L13         125 S L12 FULL
L14          94 S L12 NOT L10

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   534.91    1536.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -76.26    -112.34

FILE 'REGISTRY' ENTERED AT 19:14:14 ON 20 JUL 2009
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provided by InfoChem.

STRUCTURE FILE UPDATES:   19 JUL 2009  HIGHEST RN 1165441-73-5
DICTIONARY FILE UPDATES:  19 JUL 2009  HIGHEST RN 1165441-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10519804d.str

chain nodes :
6 7 8 9 12 13 14 15
ring nodes :
1 2 3 4 5
chain bonds :
1-7 2-12 2-14 4-6 5-13 5-15 7-8 7-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-12 4-6 5-13
exact bonds :
1-2 1-5 1-7 2-3 2-14 3-4 4-5 5-15
normalized bonds :
7-8 7-9

```
isolated ring systems :
containing 1 :


G1:Cy,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS
12:CLASS  13:CLASS  14:CLASS  15:CLASS



L15     STRUCTURE UPLOADED

=> s l15 full
FULL SEARCH INITIATED 19:14:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1817 TO ITERATE

100.0% PROCESSED     1817 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L16           0 SEA SSS FUL L15

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FULL SCREEN SEARCH COMPLETED -     1817 TO ITERATE

100.0% PROCESSED     1817 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L17           0 SEA SSS FUL L15

=> file reg
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 372.72    1909.11

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CA SUBSCRIBER PRICE                                   0.00    -112.34

FILE 'REGISTRY' ENTERED AT 19:16:36 ON 20 JUL 2009
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STRUCTURE FILE UPDATES:   19 JUL 2009  HIGHEST RN 1165441-73-5
DICTIONARY FILE UPDATES:  19 JUL 2009  HIGHEST RN 1165441-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
```

experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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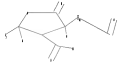

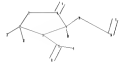

chain nodes :
6 7 8 9 12 13 14 15 16 17
ring nodes :
1 2 3 4 5
chain bonds :
1-7 2-12 2-13 4-6 5-14 5-15 7-8 7-9 15-16 16-17
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
2-12 4-6 16-17
exact bonds :
1-2 1-5 1-7 2-3 2-13 3-4 4-5 5-14 5-15 15-16
normalized bonds :
7-8 7-9
isolated ring systems :
containing 1 :

G1:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L18 STRUCTURE UPLOADED

=> s l18 full
FULL SEARCH INITIATED 19:16:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 135 TO ITERATE

100.0% PROCESSED 135 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L19 14 SEA SSS FUL L18

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 2094.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -112.34

FILE 'CAPLUS' ENTERED AT 19:17:03 ON 20 JUL 2009
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FILE COVERS 1907 - 20 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 19 Jul 2009 (20090719/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

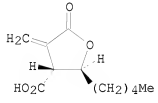
The ALL, BIB, MAX, and STD display formats in the CA/CAplus family

of databases will soon be updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> s l19 full
L20 12 L19

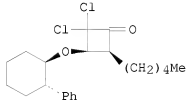
=> d ibib abs hitstr tot

L20 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:490013 CAPLUS
DOCUMENT NUMBER: 117:90013
ORIGINAL REFERENCE NO.: 117:15705a,15708a
TITLE: Novel, enantioselective lactone construction. First synthesis of methylenolactocin, antitumor antibiotic from Penicillium sp
AUTHOR(S): De Azevedo, Mariangela B. M.; Murta, Maria M.; Greene, Andrew E.
CORPORATE SOURCE: Univ. Joseph Fourier Grenoble, Grenoble, 38041, Fr.
SOURCE: Journal of Organic Chemistry (1992), 57(17), 4567-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:90013
GI



I

II



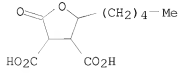
III

AB The first synthesis of (-)-methylenolactocin (I), an antitumor antibiotic isolated from the culture filtrate of Penicillium sp., was achieved from the cyclohexanol II via Baeyer-Villiger oxidation of the cyclobutanone III. The work illustrates a novel and potentially general approach to enantiopure γ-butyrolactones based on π-face differentiation in chiral olefin-ketene [2+2]-cycloaddn. The synthesis serves to confirm the structure and establish the absolute stereochem. of natural I and, also, to demonstrate a significantly improved procedure for the conversion of γ-butyrolactones to the important α-methylene derivs.

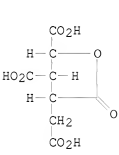
IT 142188-52-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylative methylenation of)

RN 142188-52-1 CAPLUS

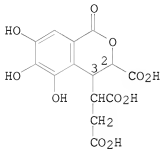
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-pentyl- (CA INDEX NAME)



L20 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:34854 CAPLUS
DOCUMENT NUMBER: 98:34854
ORIGINAL REFERENCE NO.: 98:5461a,5464a
TITLE: Phenolic constituents of Quercus valonea
AUTHOR(S): Schilling, G.; Mayer, W.
CORPORATE SOURCE: Org. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Studies in Organic Chemistry (Amsterdam) (1982), Volume Date 1981, 11(Flavonoids Bioflavonoids), 321-4
CODEN: SOCHDQ; ISSN: 0165-3253
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

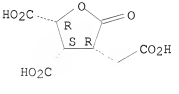


II

AB Phenolic constituents of Q. valonea are discussed. Adipic acid derivative (+)-I, which is obtained by the KMnO4 oxidation of chebulic acid (II) or trilloic acid, was synthesized in order to prove that the substituents at position 2 and 3 in II are in trans arrangement and not cis arrangement as previously claimed (J. C. Jochims, et al). Solution conformation of II is also discussed.

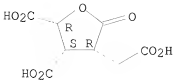
IT 79726-18-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and resolution of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone (9CI) (CA INDEX NAME)

Relative stereochemistry.

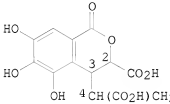


IT 79788-85-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 79788-85-5 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone, (+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



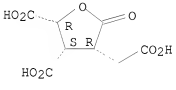
L20 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:603687 CAPLUS
DOCUMENT NUMBER: 95:203687
ORIGINAL REFERENCE NO.: 95:34029a,34032a
TITLE: Relative configuration of chebulic acid
AUTHOR(S): Schilling, Gerhard; Schweiger, Richard; Weis, Guenter; Mayer, Walter; Weiss, Johannes; Siegel, Rolf
CORPORATE SOURCE: Org. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1981), (4), 603-9
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

AB The configuration of chebulic acid (I) was examined by chemical methods, NMR, and x-ray anal.
IT 79726-18-4P 79726-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone (9CI) (CA INDEX NAME)

Relative stereochemistry.

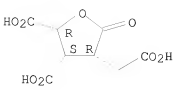


RN 79726-19-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 79788-85-5
CMF C8 H8 O8

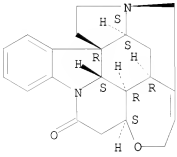
Rotation (+). Absolute stereochemistry unknown.



CM 2

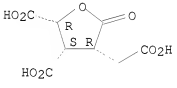
CRN 57-24-9
CMF C21 H22 N2 O2

Absolute stereochemistry. Rotation (-).



IT 79726-18-4
RL: PROC (Process)
(resolution of)
RN 79726-18-4 CAPLUS
CN Arabinaric acid, 3-carboxy-4-(carboxymethyl)-3,4-dideoxy-, 5,2-lactone
(9CI) (CA INDEX NAME)

Relative stereochemistry.

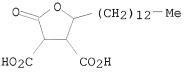


L20 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:424999 CAPLUS
DOCUMENT NUMBER: 81:24999
ORIGINAL REFERENCE NO.: 81:4041a,4044a
TITLE: Carboxylation of γ-butyrolactones with methyl methoxymagnesium carbonate. New synthesis of DL-protolichesterinic acid
AUTHOR(S): Martin, Jack; Watts, Paul C.; Johnson, Francis
CORPORATE SOURCE: East. Res. Lab., Dow Chem. U.S.A., Wayland, MA, USA
SOURCE: Journal of Organic Chemistry (1974), 39(12), 1676-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 81:24999

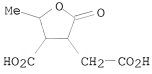
AB The carboxylation of γ-lactones at the α position is, in most cases, easily accomplished by means of Stiles' reagent (methyl methoxymagnesium carbonate). This combined with a simplified decarboxylative methylenation procedure, namely treatment of the α-carboxylactones with a mixture of formaldehyde and diethylamine, usually in a buffered acidic medium, affords a relatively simple method of synthesizing α-methylenelactones. These methods have been used in a new synthesis of dl-protolichesterinic acid.

IT 51175-46-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(decarboxylation-methylenation of)

RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



L20 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:13122 CAPLUS
DOCUMENT NUMBER: 74:13122
ORIGINAL REFERENCE NO.: 74:2117a,2120a
TITLE: Bitter principle of Jasminum primulinum. II. Structure and reactions of jasminim
AUTHOR(S): Kamikawa, Tadao; Inoue, Ken; Kubota, Tokuo; Woods, M. C.
CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, Japan
SOURCE: Tetrahedron (1970), 26(19), 4561-87
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The structure of jasminim (I, R = β-D-glucosyl), a bitter principle of J. primulinum (jasmine) based on a study of the chemical and phys. properties was confirmed by x-ray anal.
IT 30203-69-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30203-69-1 CAPLUS
CN 3-Furanacetic acid, 4-carboxytetrahydro-5-methyl-2-oxo- (CA INDEX NAME)

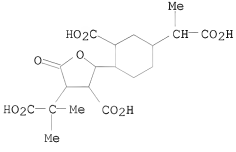


L20 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:412495 CAPLUS
DOCUMENT NUMBER: 65:12495
ORIGINAL REFERENCE NO.: 65:2306b-c
TITLE: Structure of two solanone precursors from tobacco
AUTHOR(S): Kinzer, Glenn W.; Page, Thomas F., Jr.; Johnson, Robert R.
CORPORATE SOURCE: Org. Chem. Div., Battelle Mem. Inst., Columbus, OH
SOURCE: Journal of Organic Chemistry (1966), 31(6), 1797-1800
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

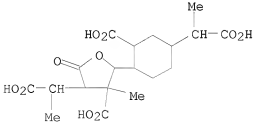
AB Two acyclic diterpenoid precursors of solanone have been isolated from tobacco and identified as diastereoisomers of 6,8-dihydroxy-11-isopropyl-4,8-dimethyl-14-oxo-4,9-pentadecadienoic acid.

IT 6619-91-6P, 3-Furanacetic acid, 4-carboxy-5-[2-carboxy-4-(1-carboxyethyl)-cyclohexyl]tetrahydro-α,α-dimethyl-2-oxo- 856818-96-7P, 2,3,4-Pentanetricarboxylic acid, 1-[2-carboxy-4-(1-carboxyethyl)cyclohexyl]-1-hydroxy-2-methyl-, γ-lactone
RL: PREP (Preparation)
(preparation of)

RN 6619-91-6 CAPLUS
CN 3-Furanacetic acid, 4-carboxy-5-[2-carboxy-4-(1-carboxyethyl)cyclohexyl]tetrahydro-α,α-dimethyl-2-oxo- (CA INDEX NAME)



RN 856818-96-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



L20 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:113136 CAPLUS
DOCUMENT NUMBER: 52:113136
ORIGINAL REFERENCE NO.: 52:19935g-i,19936a-i,19937a-h
TITLE: The synthesis of dl-protolichesterinic acid
AUTHOR(S): Van Tamelen, Eugene E.; Bach, Shirley Rosenberg
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Journal of the American Chemical Society (1958), 80, 3079-86
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:113136

AB Me dl-dihydroprotolichesterinate (180 mg.), 0.024 g. Na, and 5.5 cc. MeOH refluxed 1 hr., poured into H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, the residue (0.129 g.) dissolved in 7 cc. MeOH, the solution treated with 1 cc. H2O containing 0.0304 g. NaOH, kept 5 days at room temperature, diluted with H2O, acidified with NaHSO4, and the precipitate recrystd. from glacial AcOH, washed with petr. ether, and recrystd. again from MeOH yielded 0.056 g. neodihydroprotolichesterinic acid (I), platelets, m. 97-8° (all m.ps. are corrected) I with CH2N2 gave the Me ester, m. 38-9° (uncor.). Me dl-isodihydroprotolichesterinate (0.31 g.) and 10.5 cc. absolute MeOH refluxed 5.5 hrs. with 0.00419 g. Na, treated with 1 cc. H2O, refluxed 6.5 hrs., cooled, diluted with H2O, acidified with NaHSO4, extracted with Et2O, the extract worked up, and the residue extracted with cold petr. ether left 0.070 g. I. C13H27COCH2CO2Me (II) (5 g.) and 2.9 g. powdered NaI added to 0.41 g. Na in 10 cc. absolute MeOH, the mixture treated with cooling during 10 min. with 3.0 g. BrCH2CO2Et, kept 2 days at room temperature, filtered, the residue washed with H2O, the filtrate poured into H2O, acidified and extracted with Et2O, and the extract worked up yielded 2.53 g. dialkylation product, C25H44O7, m. 42-3°. II (10 g.), 100 cc. dry C6H6, and 10 g. pyrrolidine, b. 86.5-87° refluxed 9 hrs. with the azeotropic removal of about 0.8 cc. H2O and evaporated gave 11.5 g. pyrrolidine enamine (III) of II, yellow liquid. III (11.5 g.), 100 cc. absolute MeOH, and 5.85 g. BrCH2CO2Et refluxed 29 hrs., and stirred overnight with 20 cc. H2O, the aqueous layer extracted with Et2O, and the combined organic layer and extract evaporated gave 10 g. brown oily C13H27COCH(CO2Me)CH2CO2Et (IV); a 10-g. portion in 50 cc. absolute MeOH treated with 8 cc. 1.0M NaBH4 in MeOH, allowed to stand 3 days, treated again with 11 cc. NaBH4 solution, allowed to stand 3 hrs., poured into H2O, acidified with NaHSO4, and extracted with Et2O, the extract washed, dried, and evaporated, the residual yellow oil dissolved with 7 g. KOH in 110 cc. 90% MeOH, allowed to stand 1 day at room temperature, cooled, filtered, the residue acidified with 5% HCl, digested 1 hr. at 70°, kept several hrs. at room temperature, filtered, dried (5.1 g.), and recrystd. from C6H6 yielded 4.8 g. 3-carboxy-4-oxoheptadecanoate (V), m. 80-3°. V (1 g.) treated with CH2N2 in Et2O and evaporated yielded 1.03 g. β-carbomethoxy-γ-tridecyl-γ-butyrolactone (VI), m. 68-70° (MeOH). (EtO)2CO (80 g.) and 8.6 g. butyrolactone refluxed at 125 mm., treated during 1 hr. with 2.39 g. Na in 56 cc. absolute EtOH while removing the EtOH simultaneously with the addition, the residual pale yellow, gelatinous mass poured into 60 cc. glacial AcOH and ice and extracted with 50 cc. Et2O, and the extract worked up yielded 4.1 g. α-carbethoxy-γ-butyrolactone(VII), b0.5, 106-9°. VII in EtOH treated with excess liquid NH3 gave HO(CH2)2CH(CONH2)2, m. 152.5-53° (EtOH). VI (3 g.) and 7.55 g. (EtO)2CO treated dropwise during 1 hr. with stirring under reflux at 125 mm. with 0.212 g. Na in 5.6 cc. absolute EtOH while removing the EtOH continuously, the resulting slush poured into 6 cc. glacial AcOH and ice and extracted with Et2O, and the extract worked up yielded 3.4 g. light red oil; a 0.79-g. portion chromatographed

on 12 g. silicic acid did not give the desired carbethoxylation product; a 2.37-g. portion in 20 cc. MeOH containing 1.27 g. KOH kept 5 days at room temperature, acidified with 5% HCl, filtered, and the residue washed with H2O, dried, and extracted with ligroine (b. 60-8°) left 1.4 g. material C18H32O4, m. 133-5°. C13H27CH:CHCO2H (VIII), m. 47-9° (aqueous EtOH), was prepared by the method of Myers (C.A. 46, 1438g) and separated in 45% yield from the by-product C14H29CH(OH)CO2H by extracting the crude mixture with petr. ether at room temperature, filtering, cooling to 0°, filtering again, evaporating, and recrystg. the residue from aqueous MeOH. VIII (5 g.) in 50 cc. Et2O treated with CH2N2 in Et2O until the yellow color persisted for 5 min. and evaporated on the steam bath gave 5.3 g. Me ester (IX) of VIII. trans-VIII (1.0 g.) in a few cc. CCl4 treated with about 8 cc. 5% CCl4-Br in small portions during 0.5 hr. and evaporated, the residual yellow oily paste dissolved in 10 cc. Ac2O, the solution treated with 0.5 g. powdered KOAc, refluxed 3 hrs., treated with iced H2O, and filtered, the residual creamy paste refluxed 0.5 hr. with 15 cc. 8% alc. KOH, the mixture cooled, poured onto 50 g. ice containing a slight excess of dilute H2SO4, and extracted with Et2O, the extract evaporated, and the residual pale yellow waxy solid triturated during several days at room temperature with a few cc. petr. ether gave 0.04 g. compound A, m. 88.5-9.5°; the filtrate from the isolation of compound A cooled in ice gave 0.30 g. impure compound B, m. 56-61.5°; the crude compound B treated with three 10-cc. portions ligroine at room temperature, the combined exts. concentrated to 10 cc., cooled to 15°, and centrifuged, and the precipitate washed with a little cold ligroine and recrystd. from ligroine at 10° yielded 10 mg. pure cis-2,3-epoxyhexadecanoic acid, flakes, m. 70.0-70.9°. (CF3CO)2O (21.2 cc.), 3.5 cc. 90% H2O2, and 25 cc. CH2Cl2 added with cooling dropwise during 40 min. to 10.6 g. IX, 56.5 g. Na2HPO4, and 70 cc. dry CH2Cl2, refluxed 0.5 hr., and stirred with 100 cc. H2O, the aqueous layer washed with 70 cc. CH2Cl2, and the combined organic layer and extract washed, dried, and worked up yielded Me tridecylglycidate (X) in 3 fractions: (1) b0.4 140-6°, 3.73g.; (2) b0.4 148-50°, 2.62 g.; (3) b0.4 150-2°, 3.73 g. X (0.2902 g.), 10 cc. dioxane, and 0.5 cc. 10% aqueous NaOH refluxed 1.5 hrs. under N, cooled, poured into iced H2O containing 5 cc. 5% HCl, and extracted with Et2O, the extract worked up, and the residual oil diluted with 8 cc. petr. ether, cooled, and filtered yielded 0.122 g. trans-tridecylglycidic acid, platelets, m. 86-7°. Na (0.485 g.) in 8 cc. absolute MeOH treated with 2.79 g. CH2(CO2Me)2, the mixture treated during 10 min. with stirring with 6.00 g. X in 10 cc. absolute MeOH, refluxed 4 hrs., cooled, poured into 150 cc. ice and H2O, acidified with 5% HCl, extracted with CHCl3, and the extract worked up gave 7.85 g. crude, pale yellow, oily product which chromatographed on silicic acid gave pure α,β- dicarbomethoxy-γ-tridecyl-γ-butyrolactone (XI), white wax. XI (2.1 g.) in 40 cc. MeOH treated with 5 cc. H2O containing 1.84 g. KOH, refluxed 3 hrs., kept overnight at room temperature, decanted, the oily residue dissolved in 50 cc. H2O, the solution acidified with 5% HCl to Congo red and filtered, and the residue dried (1.182 g.) and recrystd. from 20 cc. hot MeOH yielded 0.721 g. mono-K salt (XII) of α,β-dicarboxy-γ-tridecylbutyrolactone (XIII), powder, m. 124° (decomposition); the mother liquor poured into 100 cc. H2O, acidified with 5% HCl, extracted with Et2O, and the extract worked up gave 0.494 g. white material. XII (0.0394 g.) refluxed 0.5 hr. with 0.5 cc. 5% H2SO4, cooled, extracted with Et2O, and the extract worked up gave 0.0265 g. mixed diastereoisomers of V, m. 87.5-94.5°. XII (0.050 g.) in 5

cc. MeOH acidified with 5% HCl, diluted with H2O, extracted with Et2O, and the extract dried and evaporated under N at room temperature gave 0.036 g. XIII. XII

(0.372 g.) treated with 0.207 g. Et2NH and 0.126 g. 30% aqueous CH2O, diluted with 2 cc. MeOH, heated 1 min. on the steam bath, kept 1 day at room temperature, treated again with 0.126 g. 30% aqueous CH2O, allowed to stand 1 day,

diluted with a few cc. MeOH, evaporated, the residue evaporated twice with CHCl3,

the resulting solid kept overnight in 5 cc. CHCl3 and filtered, and the residue (0.114 g.) dissolved in glacial AcOH, treated with a few drops H2O, cooled to 15°, and filtered gave 0.061 g.

dl-protolichesterinic acid (XIV), m. 92.5-4.5° the filtrate from

the crude XIV K salt evaporated, the residual semisolid dissolved in 2 cc. dry C6H6, the solution kept 3 days at room temperature with 5 cc. MeI, filtered, evaporated

at about 40° under N, the residual crude oil (0.338 g.) dissolved

in 4 cc. MeOH, the solution treated with 5.5 cc. 5% aqueous NaHCO3, allowed to stand 3 days, diluted with H2O, extracted with Et2O, the aqueous solution acidified

with 5% HCl and extracted with Et2O, and the extract worked up yielded 0.0513 g.

(crude) XIV, m. 87.5-97.5°. Crude XIV (74 mg.) chromatographed on

5 g. silicic acid gave 29% purified dl-lichesterinic acid (XV), m. 114-15°, 42% XIV, m. 100.5-101.5°, and 11.8% less pure XIV, m. 98.5-100°. XIV (30 mg.) and 5 cc. Ac2O heated 1 hr. on the steam bath, cooled, diluted with H2O, and filtered yielded 21 mg. XV, m. 113-15° (AcOH). XIV (20 mg.) in 10 cc. glacial AcOH hydrogenated

over 50 mg. 10% Pd-C, filtered, diluted with H2O, the precipitate recrystd. from

AcOH, and the product extracted with boiling ligroine and recrystd. from AcOH yielded 9 mg. dihydro derivative of XV, m. 114-16°. XII (0.3835 g.), 3 cc. MeOH, 0.079 g. Me2NH.HCl, 0.0873 g. Me2NH, and 0.097 g. 30% aqueous CH2O kept 2 days at room temperature, filtered, treated with a few cc. MeOH, evaporated

in vacuo on the steam bath, this procedure repeated twice with the addition and removal of CHCl3, the residual waxy solid treated with 3 cc. dry C6H6 and 5 cc. MeI, the mixture kept 3 days at room temperature, filtered, and the residue (0.653 g.) recrystd. from glacial AcOH yielded 0.340 g. methiodide (XVI), platelets, m. 165° (decomposition); the filtrate evaporated under N, the residual yellow oil (0.126 g.) dissolved in 2 cc. MeOH, the solution treated 3 days at room temperature with 2.1 cc. 5% aqueous NaHCO3 and extracted with

Et2O, the aqueous phase acidified with 5% HCl and extracted with Et2O, the extract

dried and evaporated, and the residue (0.038 g.) extracted with ligroine and recrystd. from aqueous AcOH gave 0.010 g. V, m. 98-100°. MeOH (5 cc.) and 2.8 cc. 5% aqueous NaHCO3 added to 0.211 g. XVI, kept 3 days at room temperature, diluted with H2O, washed with CHCl3, acidified, extracted with CHCl3, and

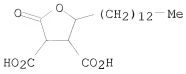
the extract worked up yielded 0.029 g. XIII, m. 92-5° (AcOH).

IT 51175-46-3 109815-40-9

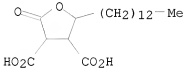
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 51175-46-3 CAPLUS

CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)



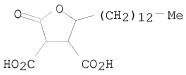
● K

L20 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:113135 CAPLUS
DOCUMENT NUMBER: 52:113135
ORIGINAL REFERENCE NO.: 52:19935a-g
TITLE: Condensation of aldehydes with esters of oxaloglycolic acid and oxalacetylglycolic acid
AUTHOR(S): Elkik, Elias
SOURCE: J. recherches centre natl. recherche sci. labs. Bellevue (Paris) (1958), No. 40, 176-96
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

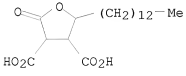
AB The preparation is given, by a modified method, of glycolic acid and also a synthesis of oxaloglycolic and oxalacetylglycolic acid esters and an infrared spectrometric study of their structures, especially of their behavior in alkaline medium. Condensation of these esters with HCHO and BzH failed to give the expected products, either in alkaline or a buffered acid medium. The ultimate objective (the conversion of oxoparaconic esters into the ene-diol structure of ascorbic acid) was not accomplished. Glycolic acid, prepared by the hydrolysis of ClCH2CO2H by BaCO3 in an autoclave for 5 hrs. with addition of 10% H2SO4 and evaporation in vacuo at a temperature lower than 70°, was esterified by EtOH and the Et glycolate converted to Et acetylglycolate, b. 84°, by AcCl. Similarly, Et benzoylglycolate, b12-14 160-5°, was obtained. Condensation of Et oxalate with either acylated ester, gave Et oxaloglycolate (I), m. 72-4°, a mixture of 2 isomers, the enediol (Ia), m. 68°, and ketol (Ib), m. 165-6°. The 2 forms were separated and studied by infrared spectroscopy, and compared with prepns. made by Fenton (C.A. 7, 332). Both Ia and Ib were unstable in strong or weak alkaline solution decomposing by hydrolysis and decarboxylation. Et oxalacetylglycolate (II), m. 93-6°, was separated into 2 isomers, the keto form, m. 100-1°, and the isomeric enediol, m. 93-4°. The mode of decomposition of these isomers by alkali at different pH with suggested mechanism was discussed. Condensations of I with HCHO or BzH in alkaline yielded only degradation products; in buffered acid medium (94 g. I in 500 cc. of aqueous solution containing 30 g. AcOH, 68 g. crystalline AcONa, and 50 cc. 30% HCHO, shaken for 5 hrs. at -10°) the product was Et methylenebisoxalacetate-H2O, m. 115-16°, identified by the dinitrophenylhydrozone, m. 158-9°. Heat converted the ester into anhydrous form, m. 83°. Condensation of II with HCHO in alkaline medium (12.5 g. II in 25 cc. H2O was treated with 6 cc. 30% HCHO and 21 g. K2CO3, shaken 6 hrs. acidified with 20 cc. 50% HCl, extracted with Et2O, washed, dried over Na2SO4, recrystd. from H2O) yielded Et oxobutyrolactonecarboxylic acid, [m. 108°; enolate, m. 255-6° (decomposition)], relatively stable at pH <9. The normal condensation product (α-oxo-β-acetoxy-β-carboxyethyl-γ-butyrolactone) was not isolated, but pyruvic acid, a product of decomposition of the latter, was isolated and characterized by its phenylhydrazone, m. 190-2°. Condensation of II with BzH in alkaline medium (12.5 g. II in 25 cc. absolute EtOH was treated with 5.4 g. BzH then 15 cc. NHEt2, stirred 6 hrs. and kept cold overnight, 50% HCl added to pH 1, extracted with Et2O, washed, recrystd. from EtOH) yielded α-oxo-β,γ-diphenyl-γ-butyrolactone, m. 212-14°, identical with that isolated by Erlenmeyer [Ber. 27, 2225 (1894)]. A mechanism was suggested showing that the first lactone formed split off phenylpyruvic acid, then was converted into the above lactone. Condensation of II in acid medium, using the method described for I, was unsuccessful; recovery of 7 g. of the original 12.5 g. of ester and only 2 g. of a viscous liquid resulted. At pH 5-6 in buffered solution condensation is not effected.

IT 5117-5-46-3 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)



L20 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:34629 CAPLUS
DOCUMENT NUMBER: 51:34629
ORIGINAL REFERENCE NO.: 51:6517c-i,6518a-d
TITLE: Preparation and properties of the isomeric forms of α-amino- and α,ε-diaminopimelic acid
AUTHOR(S): Wade, Roy; Birnbaum, Sanford M.; Winitz, Milton; Koegel, Robert J.; Greenstein, Jesse P.
CORPORATE SOURCE: Natl. Insts. of Health, Bethesda, MD
SOURCE: Journal of the American Chemical Society (1957), 79, 648-52
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 51:34629

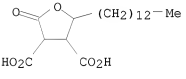
AB CH2(CH2CH2CO2Et)2 cyclized by the method of Dobson, et al., (C.A. 4, 1028) yielded 76% α-carbethoxycyclohexanone (I), b0.4 70-2°. I coupled with PhN2Cl by the method of Jackson and Manske (C.A. 25, 514) gave 60% Et H α-oxopimelate phenylhydrazone, m. 141-2° (decomposition), which saponified with 1.1N NaOH in 50% aqueous dioxane gave HO2C(CH2)4C(:NNHPh)CO2H (II), prisms, m. 141-3° (decomposition) (from EtOAc-petr. ether). II (10 g.) refluxed 6 hrs. with 15 g. Zn dust and 150 cc. 75% AcOH, filtered, and evaporated, the residue dissolved in 50 cc. H2O, treated 3 hrs. with H2S; filtered hot, and evaporated to dryness, and the crystalline residue shaken with a little EtOH and filtered gave HO2C(CH2)4CH(NH2)CO2H (III), plates, m. 216° (decomposition) (from aqueous EtOH). III (3.5 g.) in 25 cc. 2N NaOH treated at 5° with 2.2 cc. Ac2O and 20 cc. 2N NaOH in alternate portions with shaking and cooling, the mixture kept 1 hr. at room temperature, acidified to about pH 1.7 with 4N HCl and evaporated at 40° in vacuo, the residue diluted with 20 cc. H2O, the evaporation repeated, the crsyt. residue extracted with hot Me2CO, and the extract filtered, concentrated, diluted with Et2O to incipient turbidity, scratched, and filtered yielded 2.5 g. N-Ac derivative (IV) of III, m. 111-12° (from Me2CO-Et2O). IV (2.5 g.) in 100 cc. H2O adjusted to pH 7.0-7.5 with 2N LiOH, treated with 1 g. renal acylase I, diluted to 130 cc., incubated about 4 hrs. at 39°, concentrated to 50 cc. in vacuo, dialyzed 4 times against 750 cc. H2O, the combined dialyzates (3 l.) concentrated to 15 cc. in vacuo, adjusted to pH 3.4 with 6N HCl, concentrated to beginning crystallization, diluted with 50 cc. absolute EtOH, and kept 24 hrs. at room temperature gave 800 mg. L-III, [α]D26 21.5° (c 1, 5N HCl); the filtrate acidified to pH 1.7, evaporated to dryness in vacuo, and extracted with boiling Me2CO, the extract concentrated in an air stream, the residual oil refluxed 2 hrs. with 125 cc. 2N HCl and evaporated to dryness in vacuo, the residue dissolved in a little H2O, the pH adjusted to 3.4 with 2N LiOH, and the solution concentrated to beginning crystallization and diluted with absolute EtOH yielded 500 mg. D-III, [α]D26 -21.0° (c 1, 5N HCl). D- and L-III gave the following Rf values (developer, and paper given): 0.44, PhOHNH4OH, Whatman Number 4; 0.43, 4:1:5 BuOH-AcOH-H2O, Whatman Number 4; 0.73, 10:77:20 pyridine-MeOH-H2O, Whatman Number 1. A mixture of the 3 isomers of CH2[CH2CH(NH2)CO2H]2 (V) was prepared in essentially the same manner in 66% yield; it showed 2 ninhydrin-sensitive spots with Rf values 0.46 and 0.57 corresponding to meso-V and D- and L-V. V (9.5 g.) in 125 cc. 2N NaOH treated with 19.5 cc. PhCH2OCOCl in portions with cooling and stirring during about 0.5 hr., the mixture shaken 2 hrs. at room temperature and washed with EtOAc, the aqueous layer acidified to pH 1.7 with 4N

HCl, the precipitated oil extracted into EtOAc, the extract dried, concentrated to 50°
in vacuo, kept at 4° overnight, and filtered, and the filter residue recrystd. from EtOAc gave 6.0 g. di(carbobenzyloxy) derivative (VI) of DL-V, m. 164-5° with shrinking at 155°. The combined EtOAc mother liquors from VI evaporated, and the gummy residue crystallized from hot CHCl3 gave 6.2 g. meso-isomer (VII) of VI, m 123-5°. VII (30 g.) in 300 cc. AcOH and 100 cc. H2O hydrogenated over Pd black, filtered, concentrated in vacuo, diluted with 50 cc., evaporated again, and recrystd. twice from
35% aqueous EtOH yielded 7.5 g. meso-V, Rf 0.45. VI (45.8 g.) and 27.8 cc. Et3N in 600 cc. dioxane treated slowly with cooling with 24.4 cc. iso-BuCOCl below 12°, kept 1 hr. at 10°, treated dropwise with 26 cc. NH4OH(d. 0.90), allowed to stand 16 hrs., and filtered by suction yielded 18.0 g. diamide (VIII) of VI, mass of needles, m. 223-4° (from aqueous HCONMe2). VIII (21.5 g.) hydrogenolyzed in 400 cc. AcOH over Pd black, filtered, evaporated, diluted with 25 cc. H2O, and again
evaporated, the residual oil dissolved in 300 cc. H2O containing 1.15 g. Mn(OAc)2.4H2O, the pH adjusted to 6.5 with 2N LiOH, the mixture treated with 1.8 g. lyophilized amidase powder, the pH adjusted to 8.0 with 2N LiOH, diluted to 470 cc., kept 5 hrs. at 38°, concentrated to about 50 cc., dialyzed 4 times against H2O (about 900 cc. each time) at 5°, the combined dialyzates concentrated to about 50 cc. in vacuo, passed through Amberlite XE-64 (Li+ form), and collected in 20-cc. fractions, the combined fractions 19-31 evaporated to dryness, the residue dissolved in the min. amount of hot H2O, the solution treated with C, filtered, adjusted to pH 6.5 with 2N LiOH, and diluted with 4 vols. absolute EtOH, and the white amorphous precipitate reppted. twice in the same manner yielded 3.5 g. L-V, Rf 0.57, [α]D26 45.0° (c 1, N HCl). The fractions from number 176 on combined and evaporated in vacuo, the residual sirup refluxed 6 hrs. with 1 l. 3N HCl, evaporated, dissolved in 1.5N HCl, and passed through Dowex 50, and the effluent adjusted to 2.5N HCl and evaporated gave 2.9 g. D-V, [α]D26-45.5° (c 1, N HCl). The infrared absorption spectra of L-III, meso-V, and DL-V are recorded.

IT 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 109815-40-9 CAPLUS

CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)

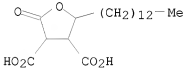


● K

L20 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1957:34628 CAPLUS
DOCUMENT NUMBER: 51:34628
ORIGINAL REFERENCE NO.: 51:6517b-c
TITLE: Synthesis of (±)-protolichesterinic acid
AUTHOR(S): Van Tamelen, E. E.; Bach, S. R.
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Chemistry & Industry (London, United Kingdom) (1956) 1308
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

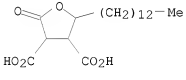
AB cf. C.A. 50, 6322a). A stereoselective synthesis of (±)-protolichesterinic acid (I) was carried out. Me 2-hexadecenoate with CF3CO3H yielded Me 2,3-epoxyhexadecanoate, b0.4 148-52°. Ring opening with di-Me malonate anion yielded, after spontaneous cyclization of the intermediate γ-hydroxy ester, α,β-dicarbomethoxy-γ-n-tridecyl-γ-butyrolactone. This on hydrolysis with hot MeOH-KOH was converted to the mono-K salt of the diacid, m. 124°, which with HCHO and Et2NH yielded I, m. 100.5-1.5°. Identification was confirmed by 3 separate tests.

IT 109815-40-9
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109815-40-9 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl-, potassium salt (1:1) (CA INDEX NAME)



● K

IT 51175-46-3, 1,1,2-Hexadecanetricarboxylic acid, 3-hydroxy-, γ-lactone
(and other derivs.)
RN 51175-46-3 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-tridecyl- (CA INDEX NAME)



L20 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1951:41362 CAPLUS
DOCUMENT NUMBER: 45:41362
ORIGINAL REFERENCE NO.: 45:7056c-i,7057a-d
TITLE: Natural tannins. V. Constitution of the "fission acid," C14H12O11, obtained from chebulinic and chebulagic acid
AUTHOR(S): Schmidt, Otto Th.; Mayer, Walter
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Annalen der Chemie, Justus Liebigs (1951), 571, 1-15
CODEN: 9X224Y
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 45, 1544d. The tri-Me derivative (I) of the "fission acid" ("Spaltsaure") (II) (cf. C.A. 44, 9176a) when neutralized and treated in aqueous EtOH with p-BrC6H4COCH2Br gave a tris(p-bromophenacyl)ester, C41H33O14Br3, micro droplets, glassy (purified by repeated solution in hot alc. and precipitation with H2O). The tris-(p-phenylphenacyl) ester, C39H48O14, forms glassy droplets. The hexa-Me derivative (III) of II on standing 2 days with MeOH-NH3 (saturated at -10°), followed by refluxing with PrOH and cooling to 0° gave trimethyl fission acid triamide, [C17H21O8N3 (IV), macroprisms, m. 257° (decomposition) (from EtOH or H2O), [α]20D 48.7 ± 3° (H2O, 20 min. after solution, c 1.9). III, b0.01 202-4°, [α]20D 49.3° (± 0.8°) (MeOH, c 2.3) prepared from I in Me2CO by treatment with CH2N2 in Et2O. Zerewitinoff detns. of "active H" in III gave very low fluctuating results [corresponding to about 0.3 mole H, indicating that the Grignard reagent reacted very sluggishly with H attached to a C atom (cf. Meunier, Bulletin society chim. (3) 29, 1177(1903)], and that no free HO groups are present in III. When I was titrated with 0.1 N NaOH (either directly or by using an excess of the reagent) 3 equivs. of alkali were used in the neutralization. However, when I was heated at 100° with an excess of 2 N NaOH, the back-titration with acid indicated the presence of a 4th CO2H group and an amorphous tetra-Na salt, C17H16O12N4 (V), was recovered by precipitation from the alkaline solution with MeOH. This behavior indicates an aromatic lactone in II. With HCl, V is reconverted into I. To 4 g. I in 60 cc. ice-cold H2O was added 40 cc. H2O, the cooled, stirred mixture treated dropwise (at temps. not above 0°) with 220 cc. N KMnO4 in the course of 10 hrs., then with another 60 cc. H2SO4, allowed to stand overnight, extracted 4 days with Et2O in a Schacherl apparatus, and the extract concentrated, treated with 25 cc. H2O, reextd. with Et2O and treated with CH2N2, giving 0.75 g. OC.CH(CH2CO2Me).CH(CO2Me).CH(CO2Me).O (VI), b0.02 150-3°, m. 81-2° (from Me2CO-H2O or C6H6-cyclohexane), [α]20D 117.5° (± 0.9°) (c 2.2, MeOH). When saponified 2 hrs. with N NaOH (or 4 hrs. with 0.1 N NaOH), followed by back titration, VI consumed 4 equivs. of alkali; the tetra-Na salt, C8H6O9N4 (VII), a neutral microcryst. hygroscopic powder precipitated from the alkaline solution with MeOH, [α]20D -4.9 ± 1° (H2O, c 1), gave rise to white, flocculent, insol. Pb, Ba, and Ag salts (but yielded no ppts. with CaCl2 or CuSO4). VII (0.9 g.) in an excess of N HCl, extracted with Et2O, gave 0.55 g. OC.CH(CH2CO2H)CH(CO2H).CH(CO2H).O (VIII), m. 200-7° (decomposition) (from Et2O), [α]20D 104.9° (± 0.7°) (c 3, H2O in 15 min.), 85.9° (after 16 days). VIII heated 1 hr. with concentrated H2SO4 or 3 hrs. with 50% H2SO4 remained unchanged. Heating VIII with PhNHMe at 186° gave no CO2. Whereas VII gave a blue color with K2Cr2O7 and HNO3, VIII gave no such coloration (cf. Fearon and Mitchell, C.A. 26, 4011). VI (0.438 g.) and MeOH-NH3 gave (after several

days at room temperature and 1 day at 0°) 0.1 g. of a tetraamide, C18H14O5N4, hexagons, m. 211° (decomposition) (from 45% EtOH), and from the mother liquors after refluxing 1 hr., 0.1 g. of the triamide lactone, C8H11O5N3 (corresponding to VIII), needles, m. 216° (decomposition) (from 80% EtOH). VI (1.01 g.) in 5 g. KOH and 5 cc. H2O was heated successively 0.5 hr. each at 100°, 180°, and 210-20°, and the cooled mixture acidified with 4 N H2SO4 and extracted with Et2O in a Schacherl apparatus, giving a mixture of 0.095 g. AcOH, and (after methylation) 0.3 g. (CO2Me)2, m. 53°, and 0.35 g. (CH2CO2Me)2 [identified as (CH2CONH2)2, m. 258°]. Isocitric acid lactone (IX), m. 162-3° (1.7 g.), treated similarly with KOH gave 1.74 mole AcOH and 0.73 mole (CO2H)2. Tricarballylic acid, m. 164°, similarly treated, was recovered unchanged. MeCH(OH)CH2CO2H on alkaline fusion yielded nearly 2 moles AcOH. These data indicate that VI cannot have the structure OC.O.CH(CO2H).C(CH2CO2H)(CO2H)CH2. O.CO.CH2.CH(CO2Me).C(CO2Me)CH2CO2Me (0.2 g.), the synthesis of which is reserved for future publication, when saponified with 5 cc. N NaOH and oxidized with 20 cc. N KMnO4 and 15 cc. N NaOH gave approx. 0.32 mole (CO2H)2 [isolated as (CO2)2Ca]. Under similar conditions 0.2 g. VI gave 2.58 moles (i.e. 65% of 4 moles) (CO2H)2. IX gave 2.32 moles, citric acid 0.24 mole, malic acid 1.7 moles, and HO2CCOCH2CO2H 1.8 moles (CO2H)2. Subjected to similar treatment, pure (CO2Na)2 remained unchanged. A mixture of 1.186 g. IV, 20 cc. and hypochlorite solution containing 0.88 g. NaOCl and
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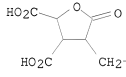
cc. 2 N NaOH was shaken 0.5 hr. and heated 15 min. on a steam bath; the excess NaOCl destroyed by solid Na2S2O3, and the mixture neutralized with AcOH and treated with NH2NHCONH2.HCl and AcONa, yielding 0.298 g. (H2NCONH)2, m. 258° (derived from NaNCO), thus indicating that the HO group involved in lactone formation in II is on an α-C atom. From various data, a structure for II is proposed.

IT 1129294-31-0P
RL: SPN (Synthetic preparation); PRP (Properties); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(Natural tannins. V. Constitution of the "fission acid," C14H12O11, obtained from chebulinic and chebulagic acid)

RN 1129294-31-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



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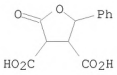
ACCESSION NUMBER: 1925:20338 CAPLUS
DOCUMENT NUMBER: 19:20338
ORIGINAL REFERENCE NO.: 19:2643d-i,2644a
TITLE: Conditions underlying the formation of unsaturated and cyclic compounds from halogenated open-chain derivatives. VII. The influence of the phenyl group on the formation of the cyclopropene ring
AUTHOR(S): Haerdi, Wilhelm; Thorpe, J. F.
SOURCE: Journal of the Chemical Society, Transactions (1925), 127, 1237-48
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB An attempt was made to prepare the acid I which, in its semi-aromatic form, would have the structure II, in order to supply further evidence in support of reported views regarding the structure of the semi-aromatic ring type of which the acid III is at present the only known member. I was not obtained but the effect of the Ph group on 3-C ring formation was studied. PhCH(CH2CO2H)2, PCl5 and Br, warmed for 2 hrs. and then poured into MeOH gave Me α-bromo-β-phenylglutarate (IV), b17 204-6°, m. 86-7°; larger amts. of Br gave the α,α'-di-Br derivative, b20 215-20°, m. 82.5-3.5°, whose Et ester (V) is a viscous liquid. The free acid m. 192-3°. Distillation of V in vacuo gives the lactone of Et α-bromo-α'-hydroxy-β-phenylglutarate, (VI), b21 230-4°. Hydrolysis of IV gave PhCH(CH2CO2H)2, when MeOH-KOH was used, or the Me ester when C5H5N was used. V (or the Me ester) and MeOH-KOH did not give the expected I but a mixture of 10% PhCH: CHCO2H and (CO2H)2 and 2-ethoxy-3-phenylcyclopropane-1,2-dicarboxylic acid, m. 198-9°, stable towards alkaline KMnO4 for 24 hrs. Me ester, b13 175-9°; Et ester, b14 184-90°. VI gave the same products but the PhCH:CHCO2H and (CO2H)2 were present in larger amts. Me 1-bromo-3-phenylcyclopropane-1,2-dicarboxylate (VII), oil which solidifies in a freezing mixture; the Br acid ester m. 175-6°. The bromination proceeds in the absence of a catalyst but in the light of an arc-lamp at 125-40°. Dibromination gave a product, C11H9O4Br(?), m. 227-8°, which may be a Br-acid or a bromolactonic acid. Hydrolysis of these esters gives phenylcyclopropanedicarboxylic acid, m. 175-6°. Et α-carbethoxy-α'-bromo-β-phenylglutaconate, on hydrolysis with aqueous KOH, gives 60-70% BzCH2CH(CO2H)2; in EtOH the hydrolysis gives BzCH2CH2CO2Et; after standing 2 days with EtOH-NH3 a compound containing both N and Br seps. PhCHBrCHBrCO2Et and CHNa(CO2Et)2 gave as the main product Et phenylcyclopropanetricarboxylate, b16 108-11°. Hydrolysis of the ester gave carboxyphenylparaconic acid (VIII), prisms with 4 H2O, m. 88°, or anhydrous, m. 187-8°; boiling with HCl gives phenylparaconic acid, m. 99-100°. PhCBr:CBrCO2Et and CHNa(CO2Et)2, condensed with 1 mol. EtONa, give an acid, C14H12O6, m. 171-2°, probably containing a lactone ring. Boiling with HCl gives phenylparaconic acid. In the absence of EtOH there results the ester EtO2CCH: CPhCBr(CO2Et)2, b16 201-5°; it reduces KMnO4 but does not react with Br in CHCl3. The ester is unchanged by the action of Na in C6H6 or PhMe; hydrolysis with 60% KOH gives VIII.
IT 861321-23-5P, 3,4-Furandicarboxylic acid, tetrahydro-2-keto-5-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 861321-23-5 CAPLUS
CN 3,4-Furandicarboxylic acid, tetrahydro-2-oxo-5-phenyl- (CA INDEX NAME)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